

# SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Frank Choi

Examiner #: 76793 Date: 3/8/01

Art Unit: 1616 Phone Number 308-2067

Serial Number: 091387135

Mail Box and Bldg/Room Location: 2D16

Results Format Preferred (circle): PAPER ~~DISK~~ ~~E-MAIL~~

If more than one search is submitted, please prioritize searches in order of need:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Method of modulating processes mediated by

Inventors (please provide full names): regulatory amino acid receptors

Nicholas D. P. Cosford, Ian A. McDonald, Stephen D. Hesse

Earliest Priority Filing Date: 8/31/99

Mark A. Vainky

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please do structure search of claims

Point of Contact:

Susan Hanley

Technical Info. Specialist

CM1 12C14 Tel: 305-4053

(1) need done 1st - structure  
search of claims not including  
language in [...]

(2) No time limit - structure  
search of claims including all  
language including language  
in [...]

Example 1  
comprehensive search

## STAFF USE ONLY

Searcher: Hanley

Searcher Phone #: \_\_\_\_\_

Searcher Location: \_\_\_\_\_

Date Searcher Picked Up: 3/15

Date Completed: 3/19

Searcher Prep & Review Time: \_\_\_\_\_

Clerical Prep Time: \_\_\_\_\_

Online Time: \_\_\_\_\_

## Type of Search

NA Sequence (#) \_\_\_\_\_

AA Sequence (#) \_\_\_\_\_

Structure (#) 1

Bibliographic \_\_\_\_\_

Litigation \_\_\_\_\_

Fulltext \_\_\_\_\_

Patent Family \_\_\_\_\_

Other \_\_\_\_\_

## Vendors and cost where applicable

STN

Dialog \_\_\_\_\_

Questel/Orbit \_\_\_\_\_

Dr. Link \_\_\_\_\_

Lexis/Nexis \_\_\_\_\_

Sequence Systems \_\_\_\_\_

WWW/Internet \_\_\_\_\_

Other (specify) \_\_\_\_\_

=&gt; d his

(FILE 'HOME' ENTERED AT 10:19:06 ON 19 MAR 2001)

FILE 'HCAPLUS' ENTERED AT 10:19:12 ON 19 MAR 2001

L1 34 S COSFORD N?/AU  
 L2 477 S MCDONALD I?/AU  
 L3 312 S HESS S?/AU  
 L4 106 S VARNEY M?/AU  
 L5 1 S L1 AND L2 AND L3 AND L4  
 L6 899 S L1-4  
 L7 457261 S AMINO ACID  
 L8 68 S L6 AND L7  
 L9 6 S L8 AND EXCIT?  
 L10 2 S L9 AND MODULAT?  
 L11 7907 S L7(4A)RECEPTOR  
 L12 6 S L11 AND L6  
 L13 7 S L10 OR L12  
 SELECT RN L13 1-7

- inventor search

FILE 'REGISTRY' ENTERED AT 10:22:59 ON 19 MAR 2001

L14 42 S E1-42

FILE 'HCAPLUS' ENTERED AT 10:23:11 ON 19 MAR 2001

L15 6 S L13 AND L14  
 L16 1 S L13 NOT L15  
 L17 21 S L11(L)HETEROCYCL?  
 L18 1008715 S ?THIO? OR ?SULFUR? OR ?MERCAPT?  
 L19 4 S L17 AND L18  
 L20 4 S L19 NOT L13  
 L21 1676 S EAA  
 L22 7 S L21(L)HETEROCYCL?  
 L23 1 S L22 AND L18  
 L24 5 S L20 OR L23  
 SELECT RN L24 1-5

selecting reg#s

for all cpds in cites 1-5 for L24

text searching

42 cpds displayed

FILE 'REGISTRY' ENTERED AT 10:32:48 ON 19 MAR 2001

L25 201 S E43-243  
 L26 200 S E244-443  
 L27 200 S E444-643  
 L28 95 S E644-738  
 L29 260 S L25-28 AND 5/SZ  
 L30 874344 S (C N S)/RELF  
 L31 0 S L29 AND L30  
 L32 19 S L29 AND 5/ELS  
 L33 0 S L25-28 AND L30

searching the cpds in L24

only 260 have a 5-membered ring

no cpds have C, N &amp; S all in the same ring

compounds that have sulfur in a ring

FILE 'HCAPLUS' ENTERED AT 10:41:59 ON 19 MAR 2001

L34 3 S L32 AND L24  
 L35 2 S L24 NOT L34

3 cites

2 cites

FILE 'REGISTRY' ENTERED AT 10:44:24 ON 19 MAR 2001

L36 3186645 S 5/SZ  
 L37 STR  
 L38 273864 S L36 AND (C S)/RELF  
 L39 435537 S L36 AND L30  
 L40 689538 S L38-39  
 L41 8 S L37 SSS SAM SUB=L40  
 L42 469760 S L40 AND C6/ESS  
 L43 SCREEN 1839 AND 2021  
 L44 8 S L43 AND L37 SSS SAM SUB=L42  
 L45 STR L37  
 L46 45 S L45 AND L43 SSS SAM SUB=L42  
 L47 1108 S L45 AND L43 SSS FUL SUB=L42  
 L48 441 S L47 AND L30  
 L49 688 S L47 AND L38

all of these cpds contain a 5-member ring

these cpds have a ring w/ only C &amp; S in ring

cpds w/ 5 member ring &amp; C, N &amp; S in ring

parent set for STR search

1108 cpds from parent search

441 cpds w/ C, N, S in a 5-member RING

688 cpds w/ only C &amp; S in a 5-member RING

FILE 'HCAPLUS' ENTERED AT 11:21:15 ON 19 MAR 2001

L50 34 S L48  
 L51 320 S L49  
 L52 0 S L50(L)(L11 OR L21)\*  
 L53 0 S L50 AND (L11 OR L21)\*  
 L54 8 S L50(L)THU/RL  
 L55 12278 S GLUTAMATE(4A)RECEPTOR  
 L56 0 S L50 AND L55\*  
 L57 26 S L50 NOT L54

8 cites for cpds w/ C, N &amp; S in 5-member ring for a medical treatment

SEARCHED BY SUSAN HANLEY 305-4053

Page 1

\* none of the cpds from L48 & L49 are in citations  
 relating to amino acid receptors

all cpds  
 have a  
 ring w/  
 only  
 C, N & S  
 as ring  
 members

L58  
L59  
L60  
L61  
L62  
L63  
L64

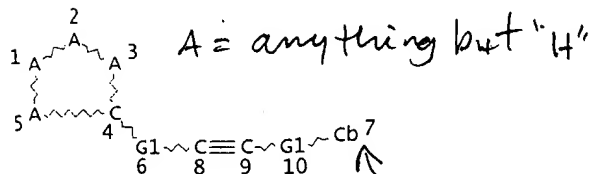
0 S L51(L)(L11 OR L21) \*  
0 S L51 AND (L11 OR L21) \*  
0 S L51 AND L55 \*  
33 S L51(L)THU/RL  
29 S L61 NOT L54  
16 S L62 AND PY>1999  
13 S L62 NOT L63

cites 12-16 only (1-11 have bad dates)  
13 cites

cpds w/ ^ c s in the 5-member ring used for a  
only medical treatment

=&gt; d que 150

L30 874344 SEA FILE=REGISTRY ABB=ON PLU=ON (C N S)/RELF  
 L36 3186645 SEA FILE=REGISTRY ABB=ON PLU=ON 5/SZ  
 L38 273864 SEA FILE=REGISTRY ABB=ON PLU=ON L36 AND (C S)/RELF  
 L39 435537 SEA FILE=REGISTRY ABB=ON PLU=ON L36 AND L30  
 L40 689538 SEA FILE=REGISTRY ABB=ON PLU=ON (L38 OR L39)  
 L42 469760 SEA FILE=REGISTRY ABB=ON PLU=ON L40 AND C6/ESS  
 L43 SCR 1839 AND 2021  
 L45 STR



REP G1=(0-20) C  
 NODE ATTRIBUTES:  
 CONNECT IS E3 RC AT 4  
 DEFAULT MLEVEL IS ATOM  
 GGCAT IS MCY UNS AT 7  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS E6 C AT 7

GRAPH ATTRIBUTES:  
 RSPEC I  
 NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L47 1108 SEA FILE=REGISTRY SUB=L42 SSS FUL L45 AND L43  
 L48 441 SEA FILE=REGISTRY ABB=ON PLU=ON L47 AND L30  
 L50 34 SEA FILE=HCAPLUS ABB=ON PLU=ON L48

STR for L45 was searched  
 against cpds w/  
 C, N, S in a 5-member ring  
 OR  
 C, N, S in a 5-member ring

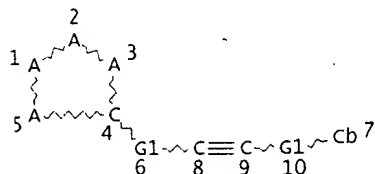
1108 cpds from search  
 cpds in L47 having rings  
 w/ C, N & S (441 cpds)



=&gt; d que 151

L30 874344 SEA FILE=REGISTRY ABB=ON PLU=ON (C N S)/RELF  
 L36 3186645 SEA FILE=REGISTRY ABB=ON PLU=ON 5/SZ  
 L38 273864 SEA FILE=REGISTRY ABB=ON PLU=ON L36 AND (C S)/RELF  
 L39 435537 SEA FILE=REGISTRY ABB=ON PLU=ON L36 AND L30  
 L40 689538 SEA FILE=REGISTRY ABB=ON PLU=ON (L38 OR L39)  
 L42 469760 SEA FILE=REGISTRY ABB=ON PLU=ON L40 AND C6/ESS  
 L43 SCR 1839 AND 2021  
 L45 STR

parent set (same as p 3)



REP G1=(0-20) C  
 NODE ATTRIBUTES:  
 CONNECT IS E3 RC AT 4  
 DEFAULT MLEVEL IS ATOM  
 GGCAT IS MCY UNS AT 7  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS E6 C AT 7

GRAPH ATTRIBUTES:  
 RSPEC I  
 NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE  
 L47 1108 SEA FILE=REGISTRY SUB=L42 SSS FUL L45 AND L43  
 L49 688 SEA FILE=REGISTRY ABB=ON PLU=ON L47 AND L38  
 L51 320 SEA FILE=HCAPLUS ABB=ON PLU=ON L49

688 cpds in L47 have a 5-member ring w/ only C & S as ring atoms

L37 ANSWER 1 OF 46 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 2002:207117 CAPLUS  
DOCUMENT NUMBER: 136:369645  
TITLE: Regiocontrolled Synthesis of Substituted Thiazoles  
AUTHOR(S): Hodgetts, Kevin J.; Kershaw, Mark T.  
CORPORATE SOURCE: Neurogen Corporation, Branford, CT, 06405, USA  
SOURCE: Organic Letters (2002), 4(8), 1363-1365  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
CLASSIFICATION: 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))

ABSTRACT:

The regiocontrolled synthesis of 2,5-disubstituted and 2,4,5-trisubstituted thiazoles from Et 2-bromo-5-chloro-4-thiazolecarboxylate using sequential palladium-catalyzed coupling reactions is described.

SUPPL. TERM: regiocontrolled synthesis thiazole coupling reaction  
INDEX TERM: Coupling reaction  
(Negishi; regiocontrolled synthesis of substituted thiazoles via Suzuki, Stille, and Negishi reactions)  
INDEX TERM: Regiochemistry  
Stille coupling reaction  
Suzuki coupling reaction  
(regiocontrolled synthesis of substituted thiazoles via Suzuki, Stille, and Negishi reactions)  
INDEX TERM: 98-80-6, Phenylboronic acid 536-74-3, Phenylacetylene  
5398-36-7 5720-06-9, 2-Methoxyphenylboronic acid  
5720-07-0, 4-Methoxyphenylboronic acid 7486-35-3,  
Tributylvinyltin 218777-23-2, 2-Pyridylzinc bromide  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(regiocontrolled synthesis of substituted thiazoles)  
INDEX TERM: 161198-41-0P 425392-44-5P 425392-45-6P 425392-46-7P  
425392-48-9P 425392-55-8P 425392-56-9P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(regiocontrolled synthesis of substituted thiazoles)  
INDEX TERM: 2104-11-2P 3704-40-3P 130161-15-8P 425392-47-8P  
425392-49-0P 425392-50-3P **425392-51-4P**  
425392-52-5P 425392-53-6P **425392-54-7P**  
425392-57-0P 425392-58-1P **425392-59-2P**  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(regiocontrolled synthesis of substituted thiazoles)  
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD.  
REFERENCE(S): (1) Bach, T; Tetrahedron Lett 2000, V41, P1707 CAPLUS  
(2) Carter, J; Biorg Med Chem Lett 1999, V9, P1167 CAPLUS  
(3) Cassar, L; J Organomet Chem 1975, V93, P253 CAPLUS  
(4) Collins, I; J Chem Soc, Perkin Trans 1 2000, P2845 CAPLUS  
(5) Dieck, H; J Organomet Chem 1975, V93, P259 CAPLUS  
(6) Hantzsch; Ber Dtsch Chem Ges 1888, V21, P942  
(7) Johnson, R; Chem Rev 1956, V56, P219 CAPLUS  
(8) Kim, H; J Heterocycl Chem 1995, V32, P937 CAPLUS

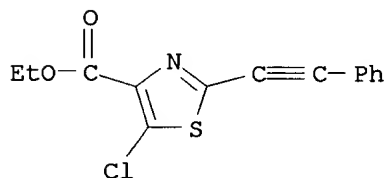
- (9) Kiryanov, A; J Org Chem 2001, V66, P7925 CAPLUS
- (10) Lewis, J; Nat Prod Rep 1996, V13, P435 CAPLUS
- (11) Li, J; Palladium in Heterocyclic Chemistry, Chapter 7  
2000, P297 CAPLUS
- (12) Metzger, J; Comprehensive Heterocyclic Chemistry 1984,  
V6, P235
- (13) Metzger, J; Thiazole and its Derivatives 1979
- (14) Miyaura, N; Chem Rev 1995, V95, P2457 CAPLUS
- (15) Negishi, E; J Org Chem 1977, V42, P1821 CAPLUS
- (16) Plouvier, B; J Heterocycl Chem 1989, V26, P1643 CAPLUS
- (17) Sakamoto, T; Chem Pharm Bull 1987, V35, P823 CAPLUS
- (18) Snieckus, V; Med Res Rev 1999, V19, P342 MEDLINE
- (19) Sonogashira, K; Tetrahedron Lett 1975, P4467 CAPLUS
- (20) South, M; J Heterocycl Chem 1991, V28, P1003 CAPLUS
- (21) Stille, J; Angew Chem 1986, V98, P504 CAPLUS
- (22) Stille, J; Pure Appl Chem 1985, V57, P1771 CAPLUS
- (23) Suzuki, A; J Organomet Chem 1999, V576, P147 CAPLUS
- (24) Takahashi, S; Synthesis 1980, P627 CAPLUS
- (25) Wiley, R; Organic Reactions 1951, V6, P367

IT 425392-51-4P 425392-54-7P 425392-59-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(regiocontrolled synthesis of substituted thiazoles)

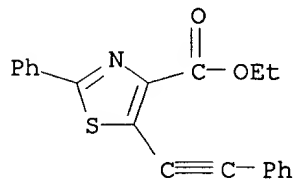
RN 425392-51-4 CAPLUS

CN 4-Thiazolecarboxylic acid, 5-chloro-2-(phenylethynyl)-, ethyl ester (9CI)  
(CA INDEX NAME)



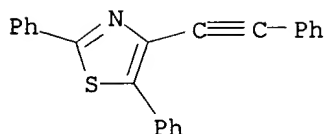
RN 425392-54-7 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-phenyl-5-(phenylethynyl)-, ethyl ester (9CI)  
(CA INDEX NAME)



RN 425392-59-2 CAPLUS

CN Thiazole, 2,5-diphenyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

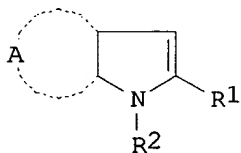


L37 ANSWER 6 OF 46 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 2001:628707 CAPLUS  
 DOCUMENT NUMBER: 135:195572  
 TITLE: Method for preparation of indole-type compounds  
 INVENTOR(S): Henkelmann, Jochem; Arndt, Jonderko  
 PATENT ASSIGNEE(S): Basf A.-G., Germany  
 SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 INT. PATENT CLASSIF.:  
     MAIN: C07D209-08  
     SECONDARY: C07D209-12; C07D209-40; C07D409-04; C07D417-04;  
                   C07B061-00  
 CLASSIFICATION: 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

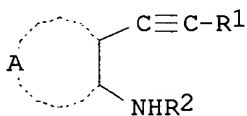
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001233855	A2	20010828	JP 2001-49221	20010223
DE 10009000	A1	20010830	DE 2000-10009000	20000225
US 2001037031	A1	20011101	US 2001-782310	20010214
US 6384235	B2	20020507		
EP 1127874	A2	20010829	EP 2001-103687	20010223

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

PRIORITY APPLN. INFO.: DE 2000-10009000 A 20000225  
 OTHER SOURCE(S): CASREACT 135:195572; MARPAT 135:195572  
 GRAPHIC IMAGE:



I



II

#### ABSTRACT:

The title compds. [I; A = hydrocarbon group which forms, together with the carbon atoms to which they are bonded, (un)substituted mono- or polycyclic arom. group optionally possessing .gtoreq.1 heteroatoms consisting of N, O, and

S; R1, R2 = H, linear or branched satd. aliph. C1-20 hydrocarbon group, linear or branched alkyl unsatd. C2-20 hydrocarbon group, optionally alkyl-substituted (un)satd. alicyclic C3-20 hydrocarbon group, or C5-20 arom. hydrocarbon group alkyl, each of which is optionally substituted and possesses .gtoreq.1 heteroatoms consisting of halo, N, P, O, S, Sn, and B in the mol. skeleton] are prepd. by cyclization of alkynylaniline or .alpha.-amino-.beta.-alkynylheterocycles (II; R1, R2 = same as above; R1, R2, or a is optionally bonded to an org. or inorg. carrier) using a Na, K, Rb, or Cs compd. in a polar aprotic solvent. This process gives substituted indoles by a simple method in high yields. Thus, a soln. of 97 mg 2-phenylethynylaniline in N-methylpyrrolidone was added to 1.05 mmol potassium tert-butoxide in 4 mL N-methylpyrrolidone and vigorously stirred at 25.degree. for 4 h to give 79% 2-phenylindole. Similarly prepd. were pyrrolopyridine, pyrrolopyrimidine, pyrroloquinoline, etc.

SUPPL. TERM: substituted indole prepn; alkynylaniline cyclization; alkynylaminoheterocycle cyclization; pyrrolopyridine pyrrolopyrimidine pyrroloquinoline prepn

INDEX TERM: Cyclization catalysts  
(alkali metal compds.; prepn. of indole-type compds. by cyclization of alkynylanilines or .alpha.-amino-.beta.-alkynylheterocycles in presence of alkali metal compd.

in

polar aprotic solvent)

INDEX TERM:

Metal alkoxides

ROLE: CAT (Catalyst use); USES (Uses)

(alkali metal; prepn. of indole-type compds. by cyclization of alkynylanilines or .alpha.-amino-.beta.-alkynylheterocycles in presence of alkali metal compd.

in

polar aprotic solvent)

INDEX TERM:

Alkali metal compounds

ROLE: CAT (Catalyst use); USES (Uses)

(alkoxides; prepn. of indole-type compds. by cyclization of alkynylanilines or .alpha.-amino-.beta.-alkynylheterocycles in presence of alkali metal compd.

in

polar aprotic solvent)

INDEX TERM:

Polar solvents

(aprotic; prepn. of indole-type compds. by cyclization

of

alkynylanilines or .alpha.-amino-.beta.-

alkynylheterocycles in presence of alkali metal compd.

in

polar aprotic solvent)

INDEX TERM:

Cyclization

Solid phase synthesis

(prepn. of indole-type compds. by cyclization of alkynylanilines or .alpha.-amino-.beta.-

alkynylheterocycles in presence of alkali metal compd.

in

polar aprotic solvent)

INDEX TERM: Alkali metal hydrides  
 Alkali metal hydroxides  
 ROLE: CAT (Catalyst use); USES (Uses)  
 (prepn. of indole-type compds. by cyclization of  
 alkynylanilines or .alpha.-amino-.beta.-  
 alkynylheterocycles in presence of alkali metal compd.  
 in  
 polar aprotic solvent)  
 INDEX TERM: 141-52-6, Sodium ethoxide 865-47-4 7646-69-7, Sodium  
 hydride 7693-26-7, Potassium hydride 21351-79-1, Cesium  
 hydroxide 23207-55-8, Calcium di-tert-butoxide  
 ROLE: CAT (Catalyst use); USES (Uses)  
 (prepn. of indole-type compds. by cyclization of  
 alkynylanilines or .alpha.-amino-.beta.-  
 alkynylheterocycles in presence of alkali metal compd.  
 in  
 polar aprotic solvent)  
 INDEX TERM: 615-43-0, 2-Iodoaniline 1066-54-2,  
 Trimethylsilylacetylene  
 3956-07-8D, 4-Iodobenzamide, MBHA resin-bound 13141-38-3,  
 2-(Phenylethynyl)aniline 52670-38-9, 2-Ethynylaniline  
 103529-16-4, 2-(Trimethylsilylethynyl)aniline 116491-50-0  
 124643-51-2 131298-21-0 209967-15-7 288254-64-8  
 288254-65-9 **288254-66-0** 288254-67-1  
 288254-68-2 288254-69-3 288254-70-6 288254-71-7  
 288254-72-8 288254-73-9 288254-74-0 288254-75-1  
 324528-81-6D, MBHA resin-bound  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. of indole-type compds. by cyclization of  
 alkynylanilines or .alpha.-amino-.beta.-  
 alkynylheterocycles in presence of alkali metal compd.  
 in  
 polar aprotic solvent)  
 INDEX TERM: 90347-86-7DP, MBHA resin-bound 357219-39-7DP, MBHA  
 resin-bound 357219-46-6DP, MBHA resin-bound  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (prepn. of indole-type compds. by cyclization of  
 alkynylanilines or .alpha.-amino-.beta.-  
 alkynylheterocycles in presence of alkali metal compd.  
 in  
 polar aprotic solvent)  
 INDEX TERM: 120-72-9P, Indole, preparation 948-65-2P, 2-Phenylindole  
 13228-37-0P, 2-Butylindole 25797-03-9P 32566-01-1P  
 52098-05-2P, 1H-Indole-2-ethanol 55463-72-4P  
 55968-16-6P, 2-(2-Thienyl)indole 78329-40-5P  
 90901-83-0P  
 258336-43-5P 288254-76-2P 288254-77-3P 288254-78-4P  
 288254-79-5P 288254-80-8P 288254-81-9P 288254-82-0P  
 357219-39-7P 357219-43-3P  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of indole-type compds. by cyclization of  
 alkynylanilines or .alpha.-amino-.beta.-  
 alkynylheterocycles in presence of alkali metal compd.  
 in

INDEX TERM: polar aprotic solvent)  
 60-29-7, Diethyl ether, uses 67-68-5, Dimethyl sulfoxide,  
 uses 68-12-2, N,N-Dimethylformamide, uses 75-21-8,  
 Ethylene oxide, uses 75-56-9, Propylene oxide, uses  
 109-99-9, Tetrahydrofuran, uses 126-33-0, Sulfolane  
 680-31-9, uses 872-50-4, N-Methylpyrrolidone, uses  
 3470-98-2, N-Butylpyrrolidone 7226-23-5  
 ROLE: NUU (Other use, unclassified); USES (Uses)  
 (reaction solvent; prepn. of indole-type compds. by  
 cyclization of alkynylanilines or .alpha.-amino-.beta.-  
 alkynylheterocycles in presence of alkali metal compd.

in

polar aprotic solvent)

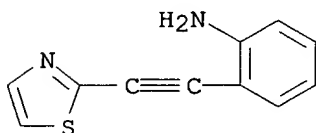
IT 288254-66-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of indole-type compds. by cyclization of alkynylanilines or  
 .alpha.-amino-.beta.-alkynylheterocycles in presence of alkali metal  
 compd. in polar aprotic solvent)

RN 288254-66-0 CAPLUS

CN Benzenamine, 2-(2-thiazolylethynyl)- (9CI) (CA INDEX NAME)



L37 ANSWER 8 OF 46 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:44710 CAPLUS

DOCUMENT NUMBER: 134:237462

TITLE: Remarkable Synthesis of

2-(Z)-6-(E)-4H-[1,4]-Thiazepin-

5-ones by Zwitterionic Rhodium-Catalyzed Chemo- and  
 Regioselective Cyclohydrocarbonylative Ring Expansion  
 of Acetylenic Thiazoles

AUTHOR(S): Van den Hoven, Bernard G.; Alper, Howard

CORPORATE SOURCE: Centre for Catalysis Research and Innovation  
 Department of Chemistry, University of Ottawa,  
 Ottawa,

ON, K1N 6N5, Can.

SOURCE: Journal of the American Chemical Society (2001),  
 123(6), 1017-1022

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 28-22 (Heterocyclic Compounds (More Than One Hetero  
 Atom))

OTHER SOURCE(S): CASREACT 134:237462

ABSTRACT:

Cyclohydrocarbonylative ring expansion of acetylenic thiazoles in the presence  
 of CO, H<sub>2</sub>, and catalytic quantities of the zwitterionic rhodium complex



(.eta.6-C6H5BPh3)-Rh+(1,5-COD) and tri-Ph phosphite affords thiazepinones in 61 to 90% yields. This novel transformation of a 5- to a 7-membered heterocycle is readily applied to acetylenic thiazoles contg. hydro, alkyl, alkyl halide, vinyl, and benzo substituents in positions 4 and 5 of the thiazole ring in addn. to alkyl-, ether-, ester-, vinyl-, and aryl-substituted alkynes at position 2.

SUPPL. TERM: cyclohydrocarbonylative ring expansion acetylenic thiazole;  
thiazepinone prepn

INDEX TERM: Chemoselectivity  
Regiochemistry  
(of zwitterionic rhodium-catalyzed  
cyclohydrocarbonylative ring expansion of acetylenic  
thiazoles)

INDEX TERM: Carbonylation  
Carbonylation catalysts  
Ring enlargement  
Ring enlargement catalysts  
(zwitterionic rhodium-catalyzed cyclohydrocarbonylative  
ring expansion of acetylenic thiazoles)

INDEX TERM: 101-02-0, Triphenyl phosphite 148538-95-8  
ROLE: CAT (Catalyst use); USES (Uses)  
(zwitterionic rhodium-catalyzed cyclohydrocarbonylative  
ring expansion of acetylenic thiazoles)

INDEX TERM: 78-80-8 95-16-9, Benzothiazole 107-19-7, Propargyl  
alcohol 137-00-8 536-74-3, Ethynylbenzene 627-41-8,  
Methyl propargyl ether 693-02-7, 1-Hexyne 693-95-8  
766-97-2, 4-Ethynyltoluene 917-92-0, tert-Butylacetylene  
1759-28-0 3034-53-5 3581-91-7 121356-98-7  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(zwitterionic rhodium-catalyzed cyclohydrocarbonylative  
ring expansion of acetylenic thiazoles)

INDEX TERM: 533-45-9P 1123-99-5P 29947-25-9P 34203-25-3P  
**35070-01-0P** 174184-05-5P 329202-28-0P  
329202-31-5P 330436-68-5P 330436-69-6P  
**330436-71-0P** 330436-72-1P 330436-73-2P  
330436-74-3P 330436-75-4P 330436-76-5P 330436-77-6P  
330436-78-7P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(zwitterionic rhodium-catalyzed cyclohydrocarbonylative  
ring expansion of acetylenic thiazoles)

INDEX TERM: 330436-79-8P 330436-80-1P 330436-81-2P 330436-82-3P  
330436-83-4P 330436-84-5P 330436-85-6P 330436-86-7P  
330436-87-8P 330436-89-0P 330436-90-3P 330436-91-4P  
330436-92-5P 330436-93-6P  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(zwitterionic rhodium-catalyzed cyclohydrocarbonylative  
ring expansion of acetylenic thiazoles)

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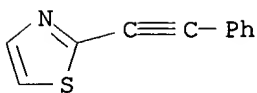
IT 35070-01-0P 330436-71-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

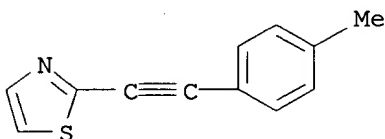
(zwitterionic rhodium-catalyzed cyclohydrocarbonylative ring expansion  
of acetylenic thiazoles)

RN 35070-01-0 CAPLUS

CN Thiazole, 2-(phenylethynyl)- (9CI) (CA INDEX NAME)



RN 330436-71-0 CAPLUS  
 CN Thiazole, 2-[(4-methylphenyl)ethynyl]- (9CI) (CA INDEX NAME)



L37 ANSWER 10 OF 46 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 2000:836580 CAPLUS  
 DOCUMENT NUMBER: 134:140937  
 TITLE: Towards rational synthesis of polar solids. Synthesis and x-ray structures of cadmium(II) meta-pyridinecarboxylate coordination polymers  
 AUTHOR(S): Evans, Owen R.; Lin, Wenbin  
 CORPORATE SOURCE: Department of Chemistry, Brandeis University, Waltham, MA, 02454, USA  
 SOURCE: Dalton (2000), (21), 3949-3954  
 CODEN: DALTFG  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 CLASSIFICATION: 78-7 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 75

ABSTRACT:  
 Two cadmium(II) coordination polymers, Cd<sub>2</sub>L<sub>14</sub>(.mu.-H<sub>2</sub>O) (1) and Cd<sub>2</sub>L<sub>24</sub>(.mu.-H<sub>2</sub>O) (2) [L<sub>1</sub> = (E)-4-(2-thiazolyl)ethenylbenzoate, L<sub>2</sub> = (E)-4-(3-pyridyl)ethenylbenzoate] based on meta-pyridinecarboxylate bridging ligands, were synthesized by the reactions of cadmium perchlorate and the corresponding benzonitrile precursor ligands under hydro(solvo)thermal conditions. Although both compds. 1 and 2 are constructed from the Cd<sub>2</sub>Ln<sub>4</sub>(.mu.-H<sub>2</sub>O) building block, x-ray single crystal structure detns. show that 1 adopts a 2-dimensional polymeric network structure while 2 exhibits a 3-dimensional framework structure as a result of the slightly different configurations of the bridging pyridinecarboxylate ligands. Owing to the presence of the bridging water mols., both 1 and 2 crystallize in centrosym. space groups.

SUPPL. TERM: crystal structure cadmium thiazolyethenylbenzoato  
 pyridylethenylbenzoato polymer; cadmium  
 thiazolyethenylbenzoate pyridylethenylbenzoate polymer  
 prepn structure; ethenylbenzoate thiazolyl pyridyl cadmium  
 polymer prepn structure; pyridinecarboxylate cadmium  
 polymer  
 prepn structure; benzoate thiazolyethenyl pyridylethenyl

cadmium polymer prepn structure

INDEX TERM: Crystal structure  
Molecular structure  
Supramolecular structure  
(of cadmium(II) (thiazolyl)ethenylbenzoato  
two-dimensional and (pyridyl)ethenylbenzoato  
three-dimensional aqua polymeric complexes)

INDEX TERM: 321696-80-4P 321696-81-5P  
ROLE: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)  
(prepn. and crystal and mol. structure of polymeric)

INDEX TERM: 500-22-1, 3-Pyridinecarbaldehyde 26104-68-7,  
(4-Cyanobenzyl)triphenylphosphonium bromide  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reactant for prepn. of cadmium(II)  
(pyridyl)ethenylbenzoato aqua three-dimensional  
polymeric  
complex)

INDEX TERM: 128587-95-1P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(reactant for prepn. of cadmium(II)  
(pyridyl)ethenylbenzoato aqua three-dimensional  
polymeric  
complex)

INDEX TERM: 3032-92-6, 4-Ethynylbenzonitrile 3034-53-5,  
2-Bromothiazole  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reactant for prepn. of cadmium(II)  
(thiazolyl)ethenylbenzoato two-dimensional polymeric  
complex)

INDEX TERM: 321696-82-6P **321696-83-7P**  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(reactant for prepn. of cadmium(II)  
(thiazolyl)ethenylbenzoato two-dimensional polymeric  
complex)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS  
RECORD.

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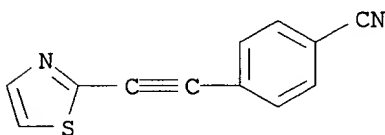
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IT 321696-83-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (reactant for prepn. of cadmium(II) (thiazolyl)ethenylbenzoato two-dimensional polymeric complex)

RN 321696-83-7 CAPLUS

CN Benzonitrile, 4-(2-thiazolylethynyl)- (9CI) (CA INDEX NAME)



L37 ANSWER 12 OF 46 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:514911 CAPLUS

DOCUMENT NUMBER: 133:252337

TITLE: Versatile indole synthesis by a 5-endo-dig cyclization

AUTHOR(S): mediated by potassium or cesium bases  
 Rodriguez, Alain Louis; Koradin, Christopher; Dohle, Wolfgang; Knochel, Paul

CORPORATE SOURCE: Department Chemie, Universitat Munchen, Munchen, 81377, Germany

SOURCE: Angewandte Chemie, International Edition (2000), 39(14), 2488-2490

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH

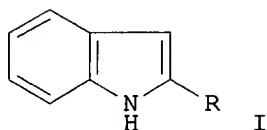
DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))

OTHER SOURCE(S): CASREACT 133:252337

GRAPHIC IMAGE:



ABSTRACT:

The combination of KOCMe<sub>3</sub>, KH, or CsOCMe<sub>3</sub> with the polar solvent NMP allows a smooth prepn. of carious indoles and azaindoles by a 5-endo-dig cyclization. Thus, cyclization of 2-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>C.tplbond.CR (R = Ph, Bu, 2-thienyl, etc.) gave indoles I in good yields.

SUPPL. TERM: indole synthesis; cyclization endo dig aniline alkyne;  
azaindole synthesis

INDEX TERM: Cyclization  
(5-endo-dig; endo-dig cyclization of alkynylanilines and  
derivs. to indoles and azaindoles mediated by potassium  
and cesium bases)

INDEX TERM: Aromatic hydrocarbons, reactions  
Aromatic hydrocarbons, reactions  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(aryl alkynes; endo-dig cyclization of alkynylanilines  
and derivs. to indoles and azaindoles mediated by  
potassium and cesium bases)

INDEX TERM: Alkynes  
Alkynes  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(aryl; endo-dig cyclization of alkynylanilines and  
derivs. to indoles and azaindoles mediated by potassium  
and cesium bases)

INDEX TERM: 865-47-4 3934-09-6, Cesium tert-butoxide 7693-26-7,  
Potassium hydride 13141-38-3 21351-79-1, Cesium  
hydroxide 52670-38-9 116491-50-0 124643-51-2  
131298-21-0 209967-15-7 288254-64-8 288254-65-9  
**288254-66-0** 288254-67-1 288254-68-2  
288254-69-3 288254-70-6 288254-71-7 288254-72-8  
288254-73-9 288254-74-0 288254-75-1  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(endo-dig cyclization of alkynylanilines and derivs. to  
indoles and azaindoles mediated by potassium and cesium  
bases)

INDEX TERM: 120-72-9P, 1H-Indole, preparation 948-65-2P 13228-37-0P  
25797-03-9P 32566-01-1P 40748-44-5P 52098-05-2P,  
1H-Indole-2-ethanol 55463-72-4P 55968-16-6P  
78329-40-5P 258336-43-5P 288254-76-2P 288254-77-3P  
288254-78-4P 288254-79-5P 288254-80-8P 288254-81-9P  
288254-82-0P  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(endo-dig cyclization of alkynylanilines and derivs. to  
indoles and azaindoles mediated by potassium and cesium  
bases)

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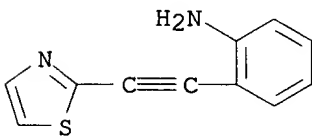
IT 288254-66-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(endo-dig cyclization of alkynylanilines and derivs. to indoles and azaindoles mediated by potassium and cesium bases)

RN 288254-66-0 CAPLUS

CN Benzenamine, 2-(2-thiazolylethynyl)- (9CI) (CA INDEX NAME)





L37 ANSWER 16 OF 46 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:733991 CAPLUS

DOCUMENT NUMBER: 132:22906

TITLE: 2-Substituted 5-acetyl-4-thiazolyl triflates as useful

building blocks for the preparation of functionalized thiazoles

AUTHOR(S): Arcadi, Antonio; Attanasi, Orazio A.; Guidi, Barbara; Rossi, Elisabetta; Santeusano, Stefania

CORPORATE SOURCE: Dipartimento Chimica, Ingegneria Chimica Materiali, Univ. L'Aquila, L'Aquila, I-67100, Italy

SOURCE: European Journal of Organic Chemistry (1999), (11), 3117-3126

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))

OTHER SOURCE(S): CASREACT 132:22906

ABSTRACT:

Readily available 2-substituted 5-acetyl-4-thiazolyl triflates (I) are useful building blocks for the prepn. of functionalized thiazoles by Pd-catalyzed cross-coupling reactions with organometallic reagents and alkoxycarbonylation and deoxygenation reactions. The combination of Pd-catalyzed coupling of I together with 1-alkynes/6-endo-dig annulation reactions in the presence of NH<sub>3</sub> leads to functionalized pyrido[3,4-c]thiazoles in satisfactory yields. The utilization of uncatalyzed displacement reactions of the triflate group represents a very simple method for the synthesis of 4-N-, 4-O-, and 4-S-substituted thiazoles.

SUPPL. TERM: thiazole prepn; thiazolyl triflate palladium catalyzed cross

INDEX TERM: coupling  
77-75-8, 3-Methyl-1-pentyn-3-ol 78-27-3,  
1-Ethynylcyclohexanol 98-80-6, Phenylboronic acid  
100-63-0, Phenylhydrazine 110-89-4, Piperidine, reactions  
110-91-8, Morpholine, reactions 536-74-3, Phenylacetylene  
629-05-0, 1-Octyne 6258-60-2,

4-Methoxybenzenemethanethiol

7486-35-3, Tributylvinylstannane 10160-87-9,  
3,3-Diethoxy-1-propyne 54663-78-4, 2-(Tributylstannyl)thiophene 87199-16-4,  
3-Formylphenylboronic acid 207397-53-3 207397-54-4  
207397-55-5 207397-56-6 207397-57-7 207397-58-8  
207397-59-9

ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of thiazoles via acetylthiazolyl triflates)

INDEX TERM: 220449-50-3P 220449-51-4P 220449-52-5P 220449-53-6P  
220449-54-7P 220449-55-8P 220449-56-9P  
**220449-57-0P** 220449-59-2P 220449-60-5P  
**220449-61-6P 220449-62-7P**  
**220449-63-8P** 220449-64-9P 220449-65-0P  
**220449-66-1P 220449-67-2P**

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. of thiazoles via acetylthiazolyl triflates)

INDEX TERM:

10045-50-8P 57560-99-3P 96497-50-6P 220449-68-3P  
220449-69-4P 220449-70-7P 220449-71-8P 220449-72-9P  
220449-73-0P 220449-74-1P 220449-75-2P 220449-76-3P  
220449-77-4P 252013-10-8P 252013-11-9P 252013-12-0P  
252013-13-1P 252013-14-2P 252013-15-3P 252013-16-4P  
252013-17-5P 252013-18-6P 252013-19-7P 252013-20-0P  
252013-21-1P 252013-22-2P

ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of thiazoles via acetylthiazolyl triflates)

REFERENCE COUNT:

66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD.

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P404

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IT 220449-57-0P 220449-61-6P 220449-62-7P

220449-63-8P 220449-66-1P 220449-67-2P

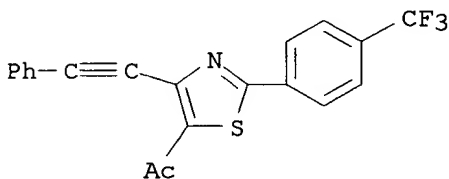
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of thiazoles via acetylthiazolyl triflates)

RN 220449-57-0 CAPLUS

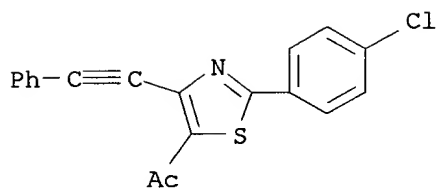
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1-[4-(phenylethynyl)-2-[4-(trifluoromethyl)phenyl]-5-thiazolyl]-  
(9CI) (CA INDEX NAME)

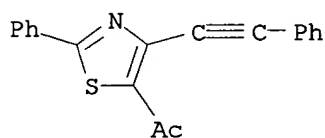


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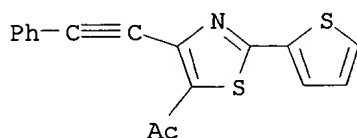
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(CA INDEX NAME)



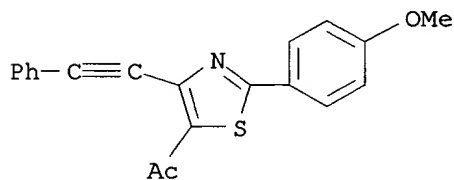
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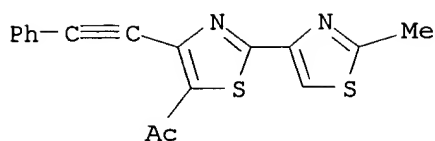
RN 220449-63-8 CAPLUS  
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RN 220449-66-1 CAPLUS  
 CN Ethanone, 1-[2-(4-methoxyphenyl)-4-(phenylethynyl)-5-thiazolyl]- (9CI) (CA INDEX NAME)



RN 220449-67-2 CAPLUS  
 CN Ethanone, 1-[2'-methyl-4-(phenylethynyl)[2,4'-bithiazol]-5-yl]- (9CI) (CA INDEX NAME)



L37 ANSWER 20 OF 46 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1999:41776 CAPLUS  
 DOCUMENT NUMBER: 130:168290  
 TITLE: Pyrido[3,4-c]thiazoles through combined  
 palladium-catalyzed coupling of 2-substituted  
 5-acetyl-4-thiazolyl triflates with

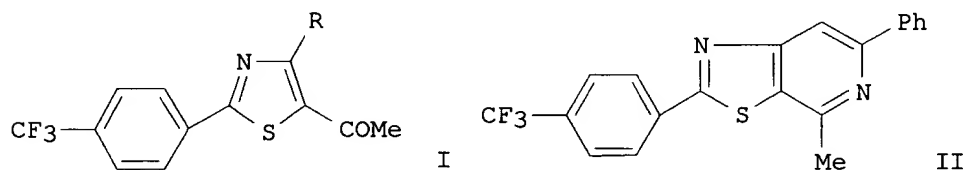
alkynes/annulation

reactions  
 AUTHOR(S): Arcadi, Antonio; Attanasi, Orazio A.; Guidi, Barbara;  
 Rossi, Elisabetta; Santeusano, Stefania  
 CORPORATE SOURCE: Dipartimento di Chimica Ingegneria Chimica e  
 Materiali

della Facoltà di Scienze, Università de L'Aquila,  
 L'Aquila, I-67100, Italy  
 SOURCE: Chemistry Letters (1999), (1), 59-60  
 CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER: Chemical Society of Japan  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 CLASSIFICATION: 28-7 (Heterocyclic Compounds (More Than One Hetero  
 Atom))

GRAPHIC IMAGE:



ABSTRACT:  
 2-Substituted 5-acetyl-4-thiazolyl triflates give in good yields  
 functionalized  
 pyrido[3,4-c]thiazoles through combined palladium-catalyzed coupling with  
 1-alkynes/6-endo-dig annulation reactions in the presence of ammonia. E.g., I  
 (R = OTf) is converted in 62% yield to I (R = C.tplbond.CPh), which is  
 converted to II in 82% yield.

SUPPL. TERM: pyridothiazole prepn; alkyne coupling annulation  
 acetylthiazolyl triflate palladium; thiazolyl triflate  
 coupling annulation alkyne palladium  
 INDEX TERM: Coupling reaction  
 Coupling reaction catalysts  
 Cyclization

(pyrido[3,4-c]thiazoles via palladium-catalyzed coupling of 5-acetyl-4-thiazolyl triflates with alkynes followed by cyclization)

INDEX TERM: Alkynes  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (pyrido[3,4-c]thiazoles via palladium-catalyzed coupling of 5-acetyl-4-thiazolyl triflates with alkynes followed by cyclization)

INDEX TERM: 14221-01-3, Tetrakis(triphenylphosphine)palladium  
 ROLE: CAT (Catalyst use); USES (Uses)  
 (pyrido[3,4-c]thiazoles via palladium-catalyzed coupling of 5-acetyl-4-thiazolyl triflates with alkynes followed by cyclization)

INDEX TERM: 207397-53-3 207397-54-4 207397-55-5 207397-56-6  
 207397-57-7 207397-58-8 207397-59-9  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (pyrido[3,4-c]thiazoles via palladium-catalyzed coupling of 5-acetyl-4-thiazolyl triflates with alkynes followed by cyclization)

INDEX TERM: 220449-50-3P 220449-51-4P 220449-52-5P 220449-53-6P  
 220449-54-7P 220449-55-8P 220449-56-9P  
**220449-57-0P** 220449-59-2P 220449-60-5P  
**220449-61-6P 220449-62-7P**  
**220449-63-8P** 220449-64-9P 220449-65-0P  
**220449-66-1P 220449-67-2P**  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (pyrido[3,4-c]thiazoles via palladium-catalyzed coupling of 5-acetyl-4-thiazolyl triflates with alkynes followed by cyclization)

INDEX TERM: 220449-68-3P 220449-69-4P 220449-70-7P 220449-71-8P  
 220449-72-9P 220449-73-0P 220449-74-1P 220449-75-2P  
 220449-76-3P 220449-77-4P  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (pyrido[3,4-c]thiazoles via palladium-catalyzed coupling of 5-acetyl-4-thiazolyl triflates with alkynes followed by cyclization)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S): (1) Alvarez-Ibarra, C; J Med Chem 1997, V40, P668 CAPLUS  
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 (15) Patt, W; Tetrahedron Lett 1997, V38, P1297 CAPLUS

- (16) Rzas, R; J Am Chem Soc 1998, V120, P591 CAPLUS
- (17) Sakamoto, T; Heterocycles 1986, V24, P2311 CAPLUS
- (18) Sakamoto, T; Heterocycles 1988, V27, P2225 CAPLUS
- (19) Sakamoto, T; Synthesis 1992, P552 CAPLUS
- (20) Schmitz, W; Tetrahedron Lett 1996, V37, P4857 CAPLUS
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IT 220449-57-0P 220449-61-6P 220449-62-7P

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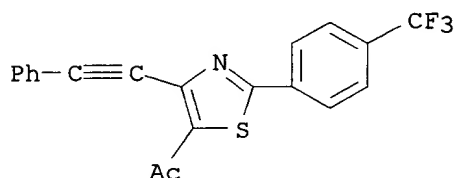
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(pyrido[3,4-c]thiazoles via palladium-catalyzed coupling of 5-acetyl-4-thiazolyl triflates with alkynes followed by cyclization)

RN 220449-57-0 CAPLUS

CN Ethanone,

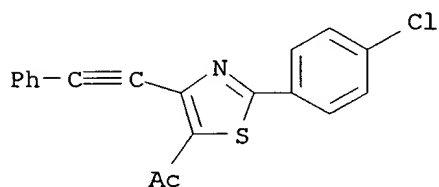
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(9CI) (CA INDEX NAME)



RN 220449-61-6 CAPLUS

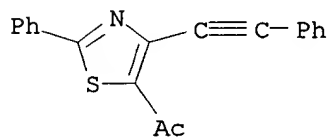
CN Ethanone, 1-[2-(4-chlorophenyl)-4-(phenylethynyl)-5-thiazolyl]- (9CI)  
(CA

INDEX NAME)



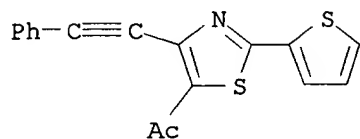
RN 220449-62-7 CAPLUS

CN Ethanone, 1-[2-phenyl-4-(phenylethynyl)-5-thiazolyl]- (9CI) (CA INDEX NAME)

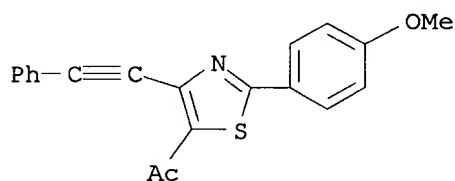




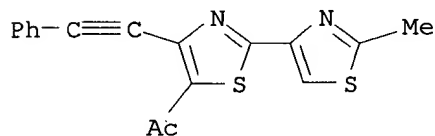
RN 220449-63-8 CAPLUS  
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INDEX NAME)



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(CA INDEX NAME)



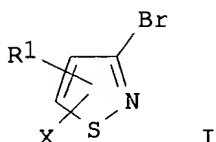
RN 220449-67-2 CAPLUS  
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(CA INDEX NAME)



L37 ANSWER 22 OF 46 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1998:272663 CAPLUS  
DOCUMENT NUMBER: 128:321593  
TITLE: Alkynylisothiazoles  
AUTHOR(S): Zlotin, S. G.; Kislitsin, P. G.; Luk'yanov, O. A.  
CORPORATE SOURCE: N. D. Zelinsky Institute of Organic Chemistry,  
Russian Academy of Sciences, Moscow, 117913, Russia  
SOURCE: Russian Chemical Bulletin (Translation of Izvestiya  
Akademii Nauk, Seriya Khimicheskaya) (1998), 47(3),  
519-523  
CODEN: RCBUEY; ISSN: 1066-5285  
PUBLISHER: Consultants Bureau  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
CLASSIFICATION: 28-7 (Heterocyclic Compounds (More Than One Hetero

Atom))

GRAPHIC IMAGE:



ABSTRACT:

A new synthesis of mono- and dialkynylisothiazoles I (R1 = 4-Br, 4-iodo, 5-H, 5-PhC.tplbond.C, X = C.tplbond.CR2, R2 = Ph, n-hexyl, CH2OH, CH2OMe) by cross-coupling of bromine- and iodine-contg. isothiazoles with terminal acetylene moieties in the PdCl2(PPh3)2-CuI-NEt3 catalytic system has been developed.

SUPPL. TERM: coupling haloisothiazole acetylene palladium;  
alkynylisothiazole prepn palladium catalyst; isothiazole  
alkynyl prepn palladium catalyst

INDEX TERM: 107-19-7, Propargyl alcohol 536-74-3, Phenylacetylene  
627-41-8 629-05-0, 1-Octyne 71091-87-7 202287-55-6  
202287-56-7

ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(palladium-catalyzed cross-coupling of haloisothiazoles  
with acetylenes)

INDEX TERM: 202287-54-5P 207000-19-9P **207000-21-3P**

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(palladium-catalyzed cross-coupling of haloisothiazoles  
with acetylenes)

INDEX TERM: 886-66-8P **207000-17-7P** 207000-18-8P  
207000-20-2P 207000-22-4P **207000-23-5P**  
**207000-24-6P** 207000-25-7P

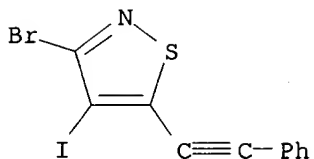
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(palladium-catalyzed cross-coupling of haloisothiazoles  
with acetylenes)

IT **207000-21-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(palladium-catalyzed cross-coupling of haloisothiazoles with  
acetylenes)

RN 207000-21-3 CAPLUS

CN Isothiazole, 3-bromo-4-iodo-5-(phenylethynyl)- (9CI) (CA INDEX NAME)

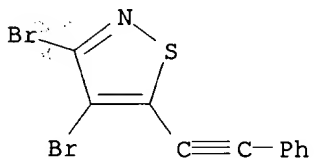


IT 207000-17-7P 207000-23-5P 207000-24-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(palladium-catalyzed cross-coupling of haloisothiazoles with  
acetylenes)

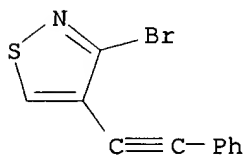
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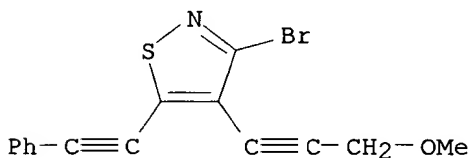
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CN Isothiazole, 3-bromo-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



RN 207000-24-6 CAPLUS

CN Isothiazole, 3-bromo-4-(3-methoxy-1-propynyl)-5-(phenylethynyl)- (9CI)  
(CA INDEX NAME)



L37 ANSWER 32 OF 46 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:507907 CAPLUS

DOCUMENT NUMBER: 121:107907

TITLE: Substituted Azole Derivatives as Nonlinear Optical  
Chromophores

AUTHOR(S): Miller, Robert D.; Lee, Victor Y.; Moylan, Christopher

CORPORATE SOURCE: R.  
Almaden Research Center, IBM, San Jose, CA, 95120-6099, USA

SOURCE: Chem. Mater. (1994), 6(7), 1023-32  
CODEN: CMATEX; ISSN: 0897-4756

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 22-13 (Physical Organic Chemistry)  
Section cross-reference(s): 73

OTHER SOURCE(S): CASREACT 121:107907

ABSTRACT:  
A series of nonlinear optical chromophores contg. a singly substituted thiazole ring has been synthesized and characterized. Selected imidazole, oxazole, and Ph analogs have also been prepd. and characterized for comparison. All exptl. hyperpolarizabilities have been extrapolated to zero frequency for purposes of comparison using the well-established two-level model. The thiazoles are superior to oxazoles and imidazoles from a nonlinear point of view. The reasons for their superiority and the implications for their use in optoelectronic devices are discussed.

SUPPL. TERM: thiazole deriv nonlinear optical chromophore; azole deriv nonlinear optical chromophore; hyperpolarizability azole deriv

INDEX TERM: Chromophores and Chromophoric systems  
(nonlinear optical, azoles, prepn. of)

INDEX TERM: Ultraviolet and visible spectra  
(of azoles)

INDEX TERM: Molecular structure-property relationship  
(hyperpolarizability, of azoles)

INDEX TERM: Optical nonlinear property  
(hyperpolarizability, of thiazole derivs.)

INDEX TERM: Heterocyclic compounds  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(nitrogen, five-membered, prepn. of, as nonlinear optical chromophores)

INDEX TERM: 4181-05-9, p-(Diphenylamino)benzaldehyde  
ROLE: RCT (Reactant)  
(Wittig reaction of, with (bromomethyl)phosphonium reagent)

INDEX TERM: 103-69-5, N-Ethylaniline  
ROLE: RCT (Reactant)  
(alkylation of, with bromohexanol)

INDEX TERM: 4286-55-9, 6-Bromo-1-hexanol  
ROLE: PRP (Properties)  
(alkylation with, of ethylaniline)

INDEX TERM: 616-47-7, N-Methylimidazole  
ROLE: RCT (Reactant)  
(bromination of)

INDEX TERM: 136517-25-4, p-(Perfluorohexylsulfonyl)bromobenzene  
ROLE: RCT (Reactant)  
(coupling of, with (methoxyphenyl)acetylene)

INDEX TERM: 156780-54-0, p-(Perfluorobutylsulfonyl)bromobenzene  
 ROLE: RCT (Reactant)  
 (coupling of, with bromoanisole)

INDEX TERM: 768-60-5, (p-Methoxyphenyl)acetylene  
 ROLE: RCT (Reactant)  
 (coupling of, with bromoazoles)

INDEX TERM: 2516-37-2, 2-Bromo-6-nitrobenzothiazole 3034-48-8,  
 2-Bromo-5-nitrothiazole 58534-03-5, 2-Bromo-5-  
 (methanesulfonyl)thiazole 101349-79-5, .beta.-Iodostyrene  
 ROLE: RCT (Reactant)  
 (coupling reaction of)

INDEX TERM: 540-37-4, p-Iodoaniline  
 ROLE: RCT (Reactant)  
 (coupling reaction of, with (trimethylsilyl)acetylene)

INDEX TERM: 536-74-3, Phenylacetylene 591-51-5, Phenyllithium  
 6303-59-9, 4-Methoxy-.beta.-bromostyrene 119950-15-1  
 ROLE: RCT (Reactant)  
 (coupling reaction of, with bromoazole)

INDEX TERM: 3034-53-5, 2-Bromothiazole  
 ROLE: RCT (Reactant)  
 (coupling reaction of, with p-bromoanisole)

INDEX TERM: 104-92-7, p-Bromoanisole  
 ROLE: RCT (Reactant)  
 (coupling reactions of, with bromoazoles)

INDEX TERM: 123-11-5, p-Methoxybenzaldehyde, reactions 7664-41-7,  
 Ammonia, reactions 13171-63-6, Tartaric acid dinitrate  
 ROLE: RCT (Reactant)  
 (cyclization of, to (methoxyphenyl)imidazole)

INDEX TERM: 121-66-4, 2-Amino-5-nitrothiazole 6285-57-0,  
 2-Amino-6-benzothiazole  
 ROLE: RCT (Reactant)  
 (diazo coupling reactions of)

INDEX TERM: 603-34-9, Triphenylamine  
 ROLE: PRP (Properties)  
 (diazo coupling with aminoazole)

INDEX TERM: 100-66-3, Anisole, reactions  
 ROLE: RCT (Reactant)  
 (diazo coupling with aminoazole)

INDEX TERM: 7727-37-9P  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (heterocyclic compounds, nitrogen, five-membered, prepn.  
 of, as nonlinear optical chromophores)

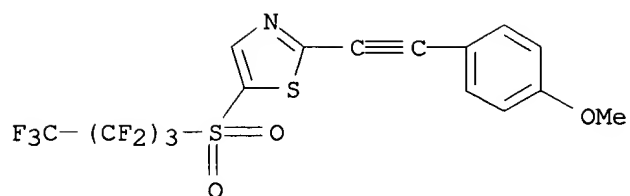
INDEX TERM: 375-72-4, Perfluorobutylsulfonyl fluoride  
 ROLE: PRP (Properties)  
 (perfluorobutylsulfonylation with, of  
 (methoxyphenyl)azoles)

INDEX TERM: 156780-53-9P, 2-(p-Methoxyphenyl)-N-methylimidazole  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (prepn. and bromination of)

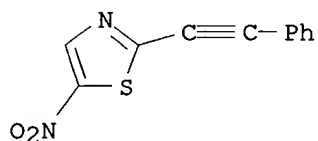
INDEX TERM: 156780-51-7P, 2-(Triethylstannyl)oxazole  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and bromodestannylation of)

INDEX TERM: 14235-81-5P, 4-Amino-1-ethynylbenzene 156780-40-4P  
 156780-42-6P 156780-43-7P

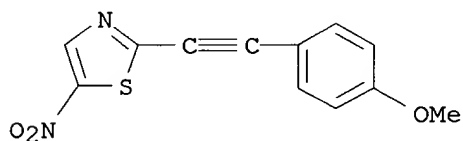
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and coupling reaction of, with bromoazole)  
 INDEX TERM: 16681-59-7P, 2-Bromo-N-methylimidazole 125533-82-6P, 2-Bromooxazole  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and coupling reaction of, with p-bromoanisole)  
 INDEX TERM: 156780-48-2P  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and diazo coupling with aminoazole)  
 INDEX TERM: 20751-78-4P 53715-66-5P 151986-01-5P 151986-03-7P  
 156780-23-3P 156780-24-4P 156780-25-5P  
**156780-29-9P** 156780-30-2P 156780-31-3P  
 156780-32-4P 156780-33-5P 156780-34-6P  
**156780-35-7P 156780-36-8P**  
**156780-37-9P 156780-38-0P** 156780-39-1P  
 156780-41-5P 156780-44-8P 156780-45-9P 156780-46-0P  
 156780-47-1P 156780-49-3P 156780-50-6P  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and linear and nonlinear optical properties of)  
 INDEX TERM: 52091-37-9P, 2-(p-Methoxyphenyl)imidazole  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and methylation of)  
 INDEX TERM: 27088-84-2P, 2-(p-Methoxyphenyl)thiazole 156780-22-2P  
**156780-26-6P** 156780-27-7P 156780-28-8P  
 156780-52-8P, 2-(p-Methoxyphenyl)oxazole  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and perfluorobutylsulfonylation of)  
 INDEX TERM: 100-10-7, p-(Dimethylamino)benzaldehyde  
 ROLE: RCT (Reactant)  
 (stereoselective Wittig reaction of, with  
 (bromomethyl)phosphonium reagent)  
 INDEX TERM: 1034-49-7, (Bromomethyl)triphenylphosphonium bromide  
 ROLE: RCT (Reactant)  
 (stereoselective Wittig reaction of, with  
 (dimethylamino)benzaldehyde)  
 INDEX TERM: 288-42-6, Oxazole  
 ROLE: PRP (Properties)  
 (triethylstannylation of)  
 IT **156780-29-9P 156780-35-7P 156780-36-8P**  
**156780-37-9P 156780-38-0P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and linear and nonlinear optical properties of)  
 RN 156780-29-9 CAPLUS  
 CN Thiazole, 2-[(4-methoxyphenyl)ethynyl]-5-[(nonafluorobutyl)sulfonyl]-  
 (9CI) (CA INDEX NAME)



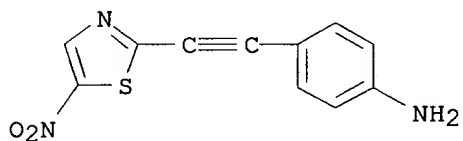
RN 156780-35-7 CAPLUS  
 CN Thiazole, 5-nitro-2-(phenylethynyl)- (9CI) (CA INDEX NAME)



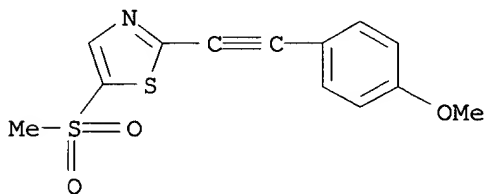
RN 156780-36-8 CAPLUS  
 CN Thiazole, 2-[(4-methoxyphenyl)ethynyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 156780-37-9 CAPLUS  
 CN Benzenamine, 4-[(5-nitro-2-thiazolyl)ethynyl]- (9CI) (CA INDEX NAME)

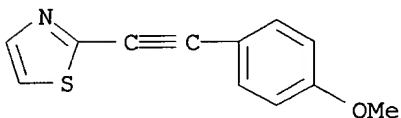


RN 156780-38-0 CAPLUS  
 CN Thiazole, 2-[(4-methoxyphenyl)ethynyl]-5-(methylsulfonyl)- (9CI) (CA INDEX NAME)





IT 156780-26-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and perfluorobutylsulfonylation of)  
 RN 156780-26-6 CAPLUS  
 CN Thiazole, 2-[(4-methoxyphenyl)ethynyl]- (9CI) (CA INDEX NAME)



L37 ANSWER 33 OF 46 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1992:214333 CAPLUS  
 DOCUMENT NUMBER: 116:214333  
 TITLE: Preparation of (arylethynyl)heteroaromatics as  
 acaricides and insecticides  
 INVENTOR(S): Rentzea, Costin; Kardorff, Uwe; Kuenast, Christoph;  
 Theobald, Hans; Kuekenhoener, Thomas  
 PATENT ASSIGNEE(S): BASF A.-G., Germany  
 SOURCE: Eur. Pat. Appl., 20 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 INT. PATENT CLASSIF.:  
 MAIN: C07D333-08  
 SECONDARY: C07D333-12; C07D333-16; C07D333-28; C07D277-22;  
 A01N043-10; A01N043-78  
 CLASSIFICATION: 27-8 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 5  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 469411	A1	19920205	EP 1991-112154	19910720
EP 469411	B1	19970611		
R: BE, CH, DE, DK, ES, FR, GB, IT, LI, NL				
DE 4024281	A1	19920206	DE 1990-4024281	19900731
ES 2103759	T3	19971001	ES 1991-112154	19910720
JP 04234381	A2	19920824	JP 1991-187421	19910726
CA 2048159	AA	19920201	CA 1991-2048159	19910730
US 5389656	A	19950214	US 1992-911386	19920713
PRIORITY APPLN. INFO.:			DE 1990-4024281	19900731
			US 1991-737866	19910730

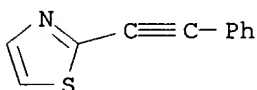
OTHER SOURCE(S): MARPAT 116:214333

ABSTRACT:

R1C.tplbond.CR2 [R1 = (substituted) heteroaryl; R2 = (substituted)  
 (polycyclic)  
 aryl] were prepd. Thus, 2-bromothiophene was condensed with PhC.tplbond.CH to  
 give 1-(2-thienyl)-2-phenylacetylene.  
 1-(3-Chloro-2-thienyl)-2-phenylacetylene  
 gave 80-100% kill of Heliothis virescens larvae on bean leaves wetted with a

400-ppm prepn.

SUPPL. TERM: heteroarom arylethynyl prepn acaricide insecticide  
INDEX TERM: Acaricides  
Insecticides  
(arylethynyl)heteroaroms.)  
INDEX TERM: 4805-17-8P **35070-01-0P** 131423-29-5P  
140918-60-1P 140918-61-2P 140918-62-3P 140918-63-4P  
140918-64-5P 140918-65-6P 140918-66-7P 140918-67-8P  
ROLE: AGR (Agricultural use); BAC (Biological activity or  
effector, except adverse); SPN (Synthetic preparation);  
BIOL  
(Biological study); PREP (Preparation); USES (Uses)  
(prepn. of, as acaricide and insecticide)  
INDEX TERM: 536-74-3, Phenylacetylene 1003-09-4, 2-Bromothiophene  
ROLE: RCT (Reactant)  
(reaction of, in prepn. of acaricides and insecticides)  
IT **35070-01-0P**  
RL: AGR (Agricultural use); BAC (Biological activity or effector, except  
adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP  
(Preparation); USES (Uses)  
(prepn. of, as acaricide and insecticide)  
RN 35070-01-0 CAPLUS  
CN Thiazole, 2-(phenylethynyl)- (9CI) (CA INDEX NAME)



L37 ANSWER 36 OF 46 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1990:235292 CAPLUS  
DOCUMENT NUMBER: 112:235292  
TITLE: Photo-activated miticidal and insecticidal  
5-ethynylthiazoles  
INVENTOR(S): Lutomski, Kathryn A.; Roush, David M.; Phillips,  
Richard B.  
PATENT ASSIGNEE(S): FMC Corp., USA  
SOURCE: U.S., 6 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
INT. PATENT CLASSIF.:  
MAIN: A01N043-78  
SECONDARY: C07D417-06; C07D277-22  
US PATENT CLASSIF.: 514365000  
CLASSIFICATION: 28-7 (Heterocyclic Compounds (More Than One Hetero  
Atom))  
Section cross-reference(s): 5  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.

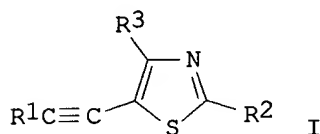
KIND DATE

APPLICATION NO. DATE

US 4889867  
OTHER SOURCE(S):  
GRAPHIC IMAGE:

A 19891226  
CASREACT 112:235292; MARPAT 112:235292

US 1988-271809 19881115



ABSTRACT:

The title compds. [I; R1 = naphthyl, Ph optionally substituted with .gtoreq.1 C1-4 alkyl, C1-4 (halo)alkoxy, halo, NO2, cyano, PhS, etc.; R2 = naphthyl, Ph optionally substituted with .gtoreq.1 C1-4 (halo)alkyl, OCF2O bridging vicinal C atoms on the Ph ring, C1-4 (halo)alkoxy, C1-4 (halo)alkylthio, No2, cyano, etc.; R3 = H, C1-4 alkyl, Ph, MeC6H4], photodynamic insecticides and acaricides, were prepd. by ethynylation of 5-iodothiazoles. Thus, a stirred mixt. of 2-(4-chlorophenyl)-5-iodothiazole (3-stop prepn. given) 0.6, PhC.tplbond.CH 0.21, (Ph3P)2PdCl2 0.013, CuI 0.9013 g, Et3N 20 mL and MeCN 10 mL

was refluxed 2 days to give 0.4 g I (R1 = Ph, R2 = 4-ClC6H4, R3 = H) which at 50 ppm gave 20% kill of Trichoplusia ni and 100% kill of Tetranychus urticae when exposed to the UV light.

SUPPL. TERM: ethynylthiazole prepn miticide insecticide; thiazole ethynyl  
prepn acaricide; ethynylation thiazole  
INDEX TERM: Acaricides  
Insecticides  
(phenylethynyl)thiazoles  
INDEX TERM: 536-74-3, Phenylacetylene  
ROLE: RCT (Reactant)  
(coupling of, with (chlorophenyl)iodothiazole, in prepn. of insecticide and acaricide)  
INDEX TERM: 7252-83-7, Bromoacetaldehyde dimethyl acetal  
ROLE: RCT (Reactant)  
(cyclocondensation of, with (chlorophenyl)thiocarboxamide, in prepn. of insecticide and acaricide)  
INDEX TERM: 17157-48-1, Bromoacetaldehyde  
ROLE: RCT (Reactant)  
(cyclocondensation of, with phenylthiocarboxamide deriv., in prepn. of insecticide and acaricide)  
INDEX TERM: 1066-54-2, Trimethylsilylacetylene  
ROLE: RCT (Reactant)  
(ethynylation by, of (trifluoromethylphenyl)iodothiazole, in prepn. of insecticide and acaricide)  
INDEX TERM: 119514-22-6P, 2-(4-Chlorophenyl)-5-iodothiazole  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation)  
 (prepn. and coupling of, with phenylethyne, in prepn. of insecticide and acaricide)

INDEX TERM: 119514-26-0P  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and coupling reaction of, with (trifluoromethylphenyl)iodothiazole, in prepn. of insecticide and acaricide)

INDEX TERM: 2521-24-6P  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and cyclocondensation of, with bromoacetaldehyde di-Me acetal, in prepn. of insecticide and acaricide)

INDEX TERM: 72505-21-6P  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and cyclocondensation of, with bromoacetaldehyde, in prepn. of insecticide and acaricide)

INDEX TERM: 119514-25-9P, 2-(4-Trifluoromethylphenyl)-5-iodothiazole  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and ethynylation of, in prepn. of insecticide and acaricide)

INDEX TERM: 27149-26-4P, 2-(4-Chlorophenyl)thiazole  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and iodination of, in prepn. of insecticide and acaricide)

INDEX TERM: 119514-24-8P, 2-(4-Trifluoromethylphenyl)thiazole  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and iodination of, in prepn. of insecticide and acaricides)

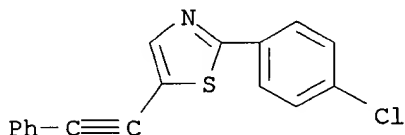
INDEX TERM: **119514-35-1P** 119514-60-2P  
 ROLE: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of, as insecticide and acaricide)

INDEX TERM: 7783-06-4P, Hydrogen sulfide, preparation  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (sulfuration by, of trifluoromethylbenzonitrile, in prepn. of insecticide and acaricide)

INDEX TERM: 619-56-7, 4-Chlorobenzamide  
 ROLE: RCT (Reactant)  
 (sulfuration of, by Lawessons's reagent, in prepn. of insecticide and acaricide)

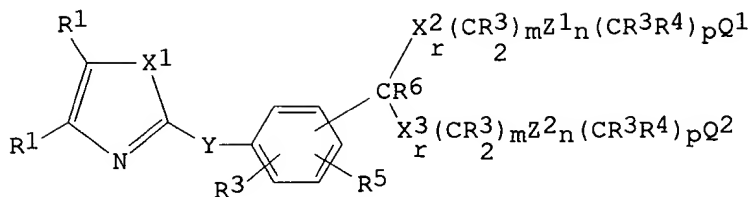
INDEX TERM: 455-18-5, 4-(Trifluoromethyl)benzonitrile  
 ROLE: RCT (Reactant)  
 (sulfuration of, by hydrogen sulfide, in prepn. of insecticide and acaricide)

IT **119514-35-1P**  
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of, as insecticide and acaricide)  
 RN 119514-35-1 CAPLUS  
 CN Thiazole, 2-(4-chlorophenyl)-5-(phenylethynyl)- (9CI) (CA INDEX NAME)



L37 ANSWER 37 OF 46 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1990:198365 CAPLUS  
 DOCUMENT NUMBER: 112:198365  
 TITLE: Preparation of heterazole dialkanoic acids as leukotriene antagonists  
 INVENTOR(S): Young, Robert N.; Atkinson, Joseph G.  
 PATENT ASSIGNEE(S): Merck Frosst Canada, Inc., Can.  
 SOURCE: Eur. Pat. Appl., 28 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 INT. PATENT CLASSIF.:  
 MAIN: C07D233-64  
 SECONDARY: C07D263-32; C07D277-22; A61K031-415; A61K031-42; A61K031-425  
 CLASSIFICATION: 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 63  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 318085	A2	19890531	EP 1988-202566	19881116
EP 318085	A3	19900314		
R: CH, DE, FR, GB, IT, LI, NL				
US 4962117	A	19901009	US 1988-265972	19881102
CA 1333801	A1	19950103	CA 1988-583725	19881122
JP 02111759	A2	19900424	JP 1988-296382	19881125
PRIORITY APPLN. INFO.:			US 1987-125622	19871125
OTHER SOURCE(S):	MARPAT 112:198365			
GRAPHIC IMAGE:				



I

# ABSTRACT:

The title compds. I [R1 = H, halo, alkyl, alkenyl, alkynyl, CF3, SR2, SOR2, SO2R2, NR32, etc.; R2 = alkyl, alkenyl, alkynyl, (un)substituted Ph, etc.; R3 = H, R2; R4 = H, halo, NO2, CN, etc.; R5 = H, halo, NO2, N3, CN, etc.; R6 = H, alkyl; X1 = NR3, O, S; X2, X3 = O, S, SO, SO2, etc.; Y = CR3;CR3, C.tplbond.C, etc.; Q1, Q2 = CO2R3, CHO, tetrazolyl, etc.; Z1, Z2 = CONR3, phenylene, pyridenylene, thiophenylene, etc.; m, p = Q, 1-8; n, n = 0, 1] are prepd. as leukotriene biosynthesis inhibitors (no data) usable as antiasthmatic, antiallergic, antiinflammatory and cytoprotective agents. A mixt. of 4-(1-methylethyl)-2-methylthiazole, isophthalaldehyde and Ac2O was refluxed to give 3-[2-[4-(1-methylethyl)-2-thiazolyl]ethenyl]benzaldehyde, which was treated with Me 3-mercaptopropanoate, N,N-dimethyl-3-mercaptopropanamide, and BF3.Et2O, in CH2Cl2, to give N,N,N',N'-tetramethyl-3,3'-[[[3-[2-[4-(1-methylethyl)-2-thiazolyl]ethenyl]phenyl]methylene]bis(thio)]bispropanamide.

SUPPL. TERM: leukotriene heterazole dialkanoate prepn; antiinflammatory heterazole dialkanoate; antiasthmatic heterazole dialkanoate; antiallergic heterazole dialkanoate

INDEX TERM: Leukotrienes

ROLE: RCT (Reactant)  
(antagonists, heterazole dialkanoic acid drugs as)

INDEX TERM: Allergy inhibitors  
Inflammation inhibitors  
(heterazole dialkanoic acid, as leukotriene inhibitors)

INDEX TERM: Bronchodilators  
(antiasthmatics, heterazole dialkanoic acid, as leukotriene inhibitors)

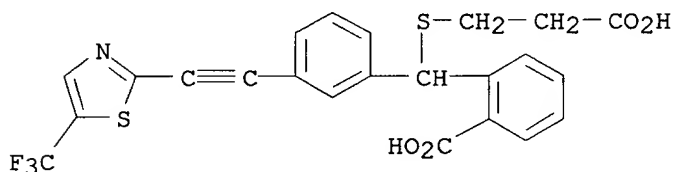
INDEX TERM: 126173-18-0P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and reaction of, with mercapto propanoates)

INDEX TERM: 126173-19-1P 126173-20-4P  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

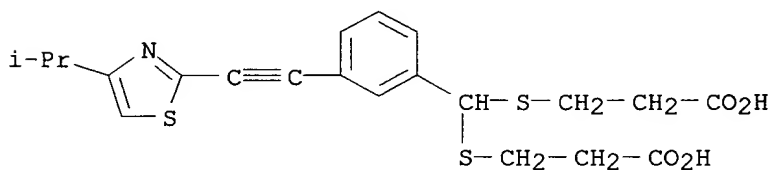
INDEX TERM: 126173-17-9P  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as leukotriene biosynthesis-inhibiting drugs)

INDEX TERM: 126173-21-5P 126173-22-6P 126173-23-7P 126173-24-8P  
126173-25-9P **126173-26-0P 126173-27-1P**  
**126173-28-2P** 126173-29-3P 126173-30-6P  
126173-31-7P 126199-19-7P

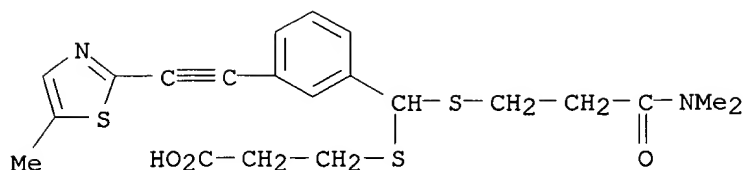
adverse);  
 ROLE: BAC (Biological activity or effector, except  
 SPN (Synthetic preparation); THU (Therapeutic use); BIOL  
 (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of, as pharmaceutical)  
 INDEX TERM: 32272-52-9  
 ROLE: RCT (Reactant)  
 (reaction of, with isoaldehyde)  
 INDEX TERM: 626-19-7, 1,3-Benzenedicarboxaldehyde  
 ROLE: RCT (Reactant)  
 (reaction of, with thiazole deriv.)  
 INDEX TERM: 2935-90-2, Methyl 3-mercaptopropanoate 92065-71-9  
 ROLE: RCT (Reactant)  
 (reaction of, with thiazolylolethynylbenzaldehyde deriv.)  
 IT 126173-26-0P 126173-27-1P 126173-28-2P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic  
 preparation); THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)  
 (prepn. of, as pharmaceutical)  
 RN 126173-26-0 CAPLUS  
 CN Benzoic acid, 2-[[[(2-carboxyethyl)thio][3-[[5-(trifluoromethyl)-2-  
 thiazolyl]ethynyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



RN 126173-27-1 CAPLUS  
 CN Propanoic acid, 3,3'-[[[3-[[4-(1-methylethyl)-2-  
 thiazolyl]ethynyl]phenyl]methylene]bis(thio)]bis- (9CI) (CA INDEX NAME)



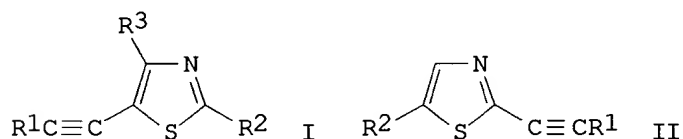
RN 126173-28-2 CAPLUS  
 CN Propanoic acid, 3-[[[3-(dimethylamino)-3-oxopropyl]thio][3-[(5-methyl-2-  
 thiazolyl)ethynyl]phenyl]methyl]thio]- (9CI) (CA INDEX NAME)



L37 ANSWER 38 OF 46 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1989:135230 CAPLUS  
 DOCUMENT NUMBER: 110:135230  
 TITLE: Preparation of ethynylthiazoles as photodynamic insecticides and acaricides  
 INVENTOR(S): Lutomski, Kathryn A.; Roush, David M.; Phillips, Richard B.  
 PATENT ASSIGNEE(S): FMC Corp., USA  
 SOURCE: U.S., 7 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 INT. PATENT CLASSIF.:  
 MAIN: C07D417-06  
 SECONDARY: C07D277-22; A01N043-78  
 US PATENT CLASSIF.: 514365000  
 CLASSIFICATION: 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 5  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4788207	A	19881129	US 1988-161867	19880229

OTHER SOURCE(S): CASREACT 110:135230; MARPAT 110:135230  
 GRAPHIC IMAGE:



ABSTRACT:  
 Thirty-nine title 5-ethynylthiazoles I [R1 = C1-6 alkyl, methylthienyl, Me3Si, (un)substituted Ph; R2 = (un)substituted Ph, thienyl; R3 = H, C1-4 alkyl, Ph, MeC6H4] and nine isomeric 2-ethynylthiazoles II [R1 = Ph, alkylthienyl; R2 = (methyl)thienyl, trialkylstannyl, (un)substituted Ph] were prepd. as photoactivated miticides and insecticides. 4-ClC6H4CONH2 was sulfurated by refluxing 2 h in PhMe with Lawesson's reagent and cyclocondensed with BrCH2CH(OMe)2 by refluxing .apprx.3 days in EtOH in the presence of concd. HCl to give 2-(4-chlorophenyl)thiazole. The latter was metalated with BuLi at



-78.degree.C in Et2O and treated with 1,2-diiodoethane to give the corresponding 5-iodothiazole which was refluxed 2 days with PhC.tplbond.CH in MeCN in the presence of Et3N, [Ph3P] PdCl2, and CuI to give I (R1 = Ph, R2 = 4-ClC6H4; R3 = H) (III). At 50 ppm III gave 100% kill of Tetranychus urticae and 20% kill of Trichoplusia ni after 48 h UV light exposure.

SUPPL. TERM: ethynylthiazole prepn miticide insecticide photosensitized  
INDEX TERM: Acaricides

Insecticides

(ethynylthiazoles)

INDEX TERM: 624-31-7P 2521-24-6P 3034-53-5P 27149-26-4P  
42140-95-4P 72505-21-6P 119514-22-6P 119514-23-7P  
119514-24-8P 119514-25-9P 119514-26-0P 119514-28-2P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation)

(prepn. and reaction of, in prepn. of insecticides and  
acaricides)

INDEX TERM: 119514-10-2P 119514-11-3P 119514-12-4P  
119514-13-5P 119514-14-6P 119514-15-7P  
119514-16-8P 119514-17-9P  
119514-18-0P 119514-19-1P 119514-20-4P  
119514-21-5P 119514-28-2P 119514-29-3P  
119514-30-6P 119514-31-7P  
119514-32-8P 119514-33-9P  
119514-34-0P 119514-35-1P  
119514-36-2P 119514-37-3P  
119514-38-4P 119514-39-5P  
119514-40-8P 119514-41-9P  
119514-42-0P 119514-43-1P  
119514-44-2P 119514-45-3P  
119514-46-4P 119514-47-5P  
119514-48-6P 119514-49-7P  
119514-50-0P 119514-51-1P  
119514-52-2P 119514-53-3P  
119514-54-4P 119514-55-5P  
119514-56-6P 119514-57-7P 119514-58-8P  
119514-59-9P 119514-60-2P 119514-61-3P  
119539-82-1P

ROLE: AGR (Agricultural use); BAC (Biological activity or  
effector, except adverse); SPN (Synthetic preparation);

BIOL

(Biological study); PREP (Preparation); USES (Uses)  
(prepn. of, as insecticide and acaricide)

INDEX TERM: 455-18-5, 4-(Trifluoromethyl)benzonitrile 536-74-3,  
Phenylacetylene 541-41-3, Ethyl chloroformate 619-56-7,  
4-Chlorobenzamide 624-73-7, 1,2-Diiodoethane 1066-54-2,  
(Trimethylsilyl)acetylene 5813-89-8, 2-  
Thiophenecarboxamide 7252-83-7, Bromoacetaldehyde

dimethyl

acetal 16494-36-3, 2-Iodo-5-methylthiophene 17157-48-1,  
Bromoacetaldehyde 119514-27-1, 2-[(5-Methyl-2-  
thienyl)ethynyl]thiazole

ROLE: RCT (Reactant)

(reaction of, in prepn. of insecticides and acaricides)

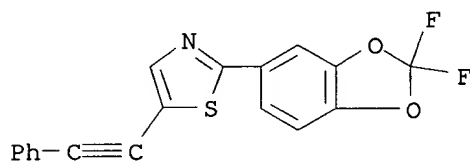
IT 119514-11-3P 119514-12-4P 119514-14-6P

119514-15-7P 119514-16-8P 119514-17-9P  
 119514-18-0P 119514-29-3P 119514-30-6P  
 119514-31-7P 119514-32-8P 119514-33-9P  
 119514-34-0P 119514-35-1P 119514-36-2P  
 119514-37-3P 119514-38-4P 119514-39-5P  
 119514-40-8P 119514-41-9P 119514-42-0P  
 119514-43-1P 119514-44-2P 119514-45-3P  
 119514-46-4P 119514-47-5P 119514-48-6P  
 119514-49-7P 119514-50-0P 119514-51-1P  
 119514-52-2P 119514-53-3P 119514-54-4P  
 119514-55-5P 119514-56-6P 119514-57-7P  
 119539-82-1P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of, as insecticide and acaricide)

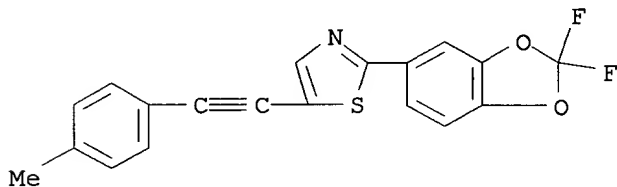
RN 119514-11-3 CAPLUS

CN Thiazole, 2-(2,2-difluoro-1,3-benzodioxol-5-yl)-5-(phenylethynyl)- (9CI)  
 (CA INDEX NAME)



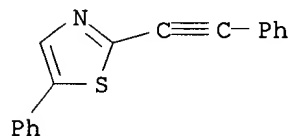
RN 119514-12-4 CAPLUS

CN Thiazole, 2-(2,2-difluoro-1,3-benzodioxol-5-yl)-5-[(4-methylphenyl)ethynyl]- (9CI) (CA INDEX NAME)



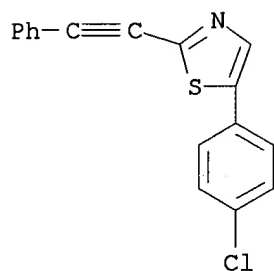
RN 119514-14-6 CAPLUS

CN Thiazole, 5-phenyl-2-(phenylethynyl)- (9CI) (CA INDEX NAME)



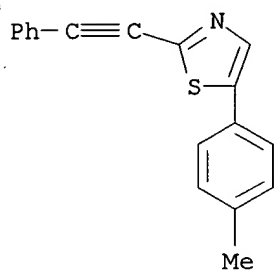
RN 119514-15-7 CAPLUS

CN Thiazole, 5-(4-chlorophenyl)-2-(phenylethynyl)- (9CI) (CA INDEX NAME)



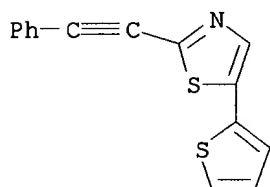
RN 119514-16-8 CAPLUS

CN Thiazole, 5-(4-methylphenyl)-2-(phenylethynyl)- (9CI) (CA INDEX NAME)



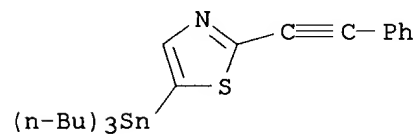
RN 119514-17-9 CAPLUS

CN Thiazole, 2-(phenylethynyl)-5-(2-thienyl)- (9CI) (CA INDEX NAME)



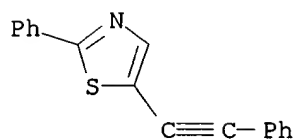
RN 119514-18-0 CAPLUS

CN Thiazole, 2-(phenylethynyl)-5-(tributylstannyl)- (9CI) (CA INDEX NAME)

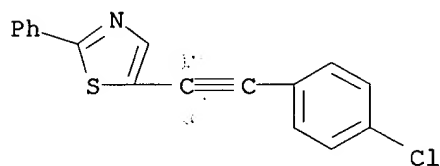


RN 119514-29-3 CAPLUS

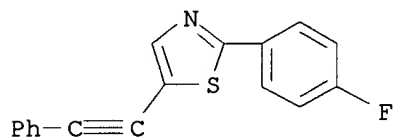
CN Thiazole, 2-phenyl-5-(phenylethynyl)- (9CI) (CA INDEX NAME)



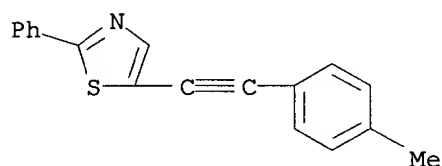
RN 119514-30-6 CAPLUS  
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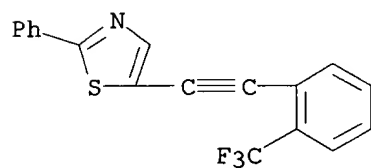
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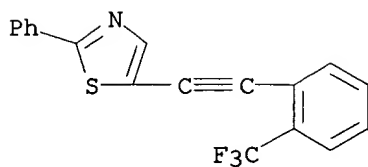


RN 119514-32-8 CAPLUS  
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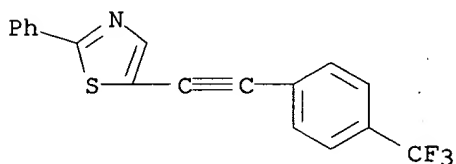


RN 119514-33-9 CAPLUS  
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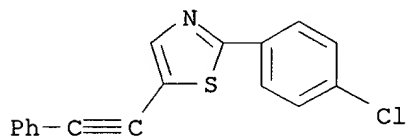




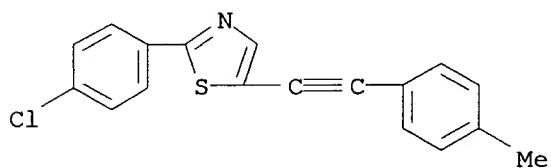
RN 119514-34-0 CAPLUS  
 CN Thiazole, 2-phenyl-5-[[4-(trifluoromethyl)phenyl]ethynyl]- (9CI) (CA INDEX NAME)



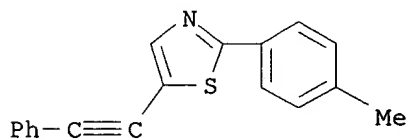
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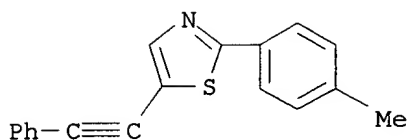


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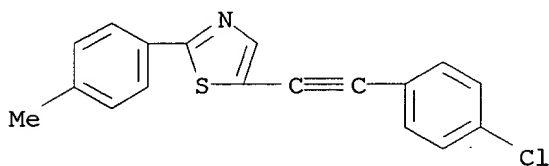


RN 119514-37-3 CAPLUS  
 CN Thiazole, 2-(4-methylphenyl)-5-(phenylethynyl)- (9CI) (CA INDEX NAME)

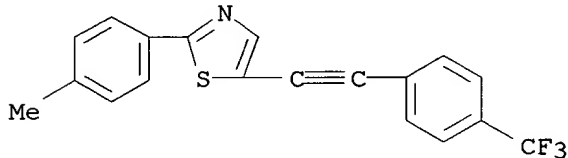




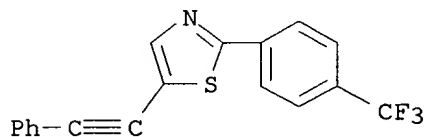
RN 119514-38-4 CAPLUS  
 CN Thiazole, 5-[(4-chlorophenyl)ethynyl]-2-(4-methylphenyl)- (9CI) (CA  
 INDEX  
 NAME)



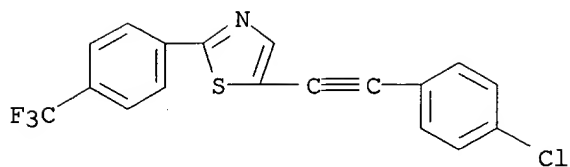
RN 119514-39-5 CAPLUS  
 CN Thiazole, 2-(4-methylphenyl)-5-[[4-(trifluoromethyl)phenyl]ethynyl]-  
 (9CI)  
 (CA INDEX NAME)



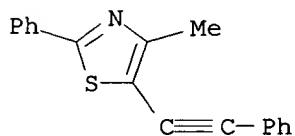
RN 119514-40-8 CAPLUS  
 CN Thiazole, 5-(phenylethynyl)-2-[4-(trifluoromethyl)phenyl]- (9CI) (CA  
 INDEX NAME)



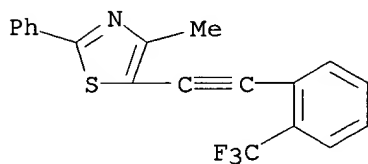
RN 119514-41-9 CAPLUS  
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 (9CI)  
 (CA INDEX NAME)



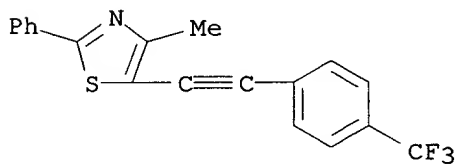
RN 119514-42-0 CAPLUS  
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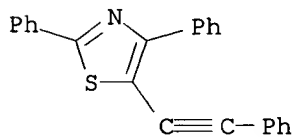
RN 119514-43-1 CAPLUS  
 CN Thiazole, 4-methyl-2-phenyl-5-[[2-(trifluoromethyl)phenyl]ethynyl]- (9CI)  
 (CA INDEX NAME)



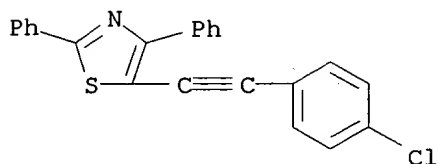
RN 119514-44-2 CAPLUS  
 CN Thiazole, 4-methyl-2-phenyl-5-[[4-(trifluoromethyl)phenyl]ethynyl]- (9CI)  
 (CA INDEX NAME)



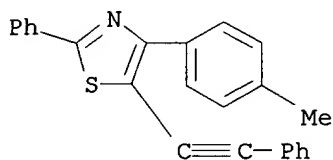
RN 119514-45-3 CAPLUS  
 CN Thiazole, 2,4-diphenyl-5-(phenylethynyl)- (9CI) (CA INDEX NAME)



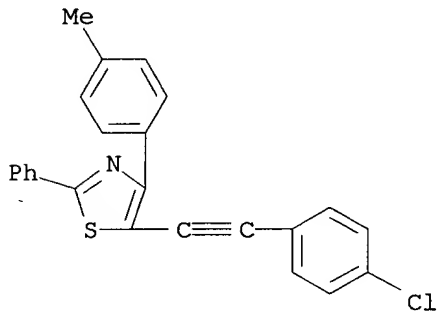
RN 119514-46-4 CAPLUS  
 CN Thiazole, 5-[(4-chlorophenyl)ethynyl]-2,4-diphenyl- (9CI) (CA INDEX NAME)



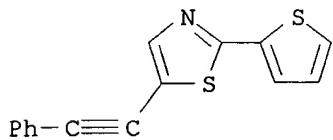
RN 119514-47-5 CAPLUS  
 CN Thiazole, 4-(4-methylphenyl)-2-phenyl-5-(phenylethynyl)- (9CI) (CA INDEX NAME)



RN 119514-48-6 CAPLUS  
 CN Thiazole, 5-[(4-chlorophenyl)ethynyl]-4-(4-methylphenyl)-2-phenyl- (9CI) (CA INDEX NAME)

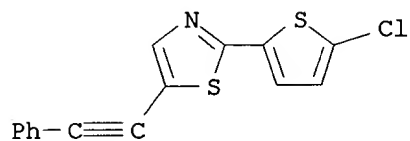


RN 119514-49-7 CAPLUS  
 CN Thiazole, 5-(phenylethynyl)-2-(2-thienyl)- (9CI) (CA INDEX NAME)

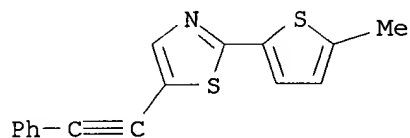




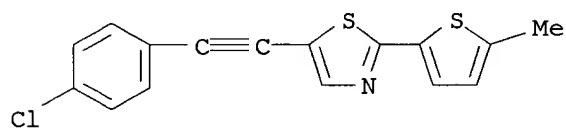
RN 119514-50-0 CAPLUS  
 CN Thiazole, 2-(5-chloro-2-thienyl)-5-(phenylethynyl)- (9CI) (CA INDEX NAME)



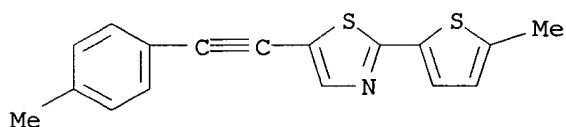
RN 119514-51-1 CAPLUS  
 CN Thiazole, 2-(5-methyl-2-thienyl)-5-(phenylethynyl)- (9CI) (CA INDEX NAME)



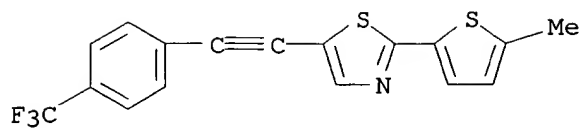
RN 119514-52-2 CAPLUS  
 CN Thiazole, 5-[(4-chlorophenyl)ethynyl]-2-(5-methyl-2-thienyl)- (9CI) (CA INDEX NAME)



RN 119514-53-3 CAPLUS  
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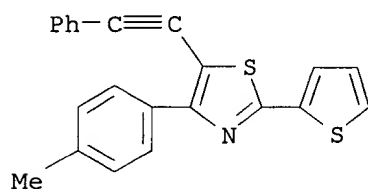


RN 119514-54-4 CAPLUS  
 CN Thiazole, 2-(5-methyl-2-thienyl)-5-[[4-(trifluoromethyl)phenyl]ethynyl]- (9CI) (CA INDEX NAME)



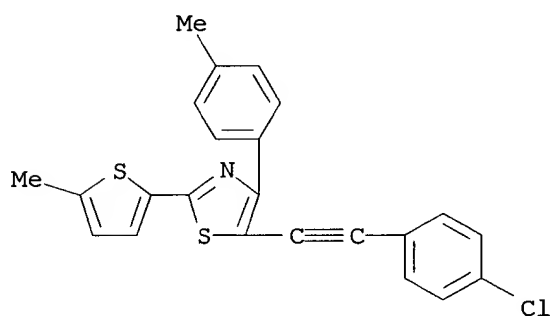
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CN Thiazole, 4-(4-methylphenyl)-5-(phenylethynyl)-2-(2-thienyl)- (9CI) (CA INDEX NAME)



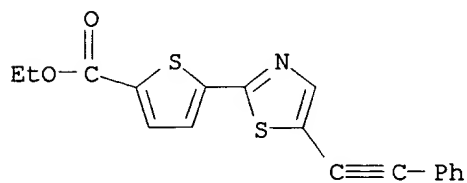
RN 119514-56-6 CAPLUS

CN Thiazole, 5-[(4-chlorophenyl)ethynyl]-4-(4-methylphenyl)-2-(5-methyl-2-thienyl)- (9CI) (CA INDEX NAME)



RN 119514-57-7 CAPLUS

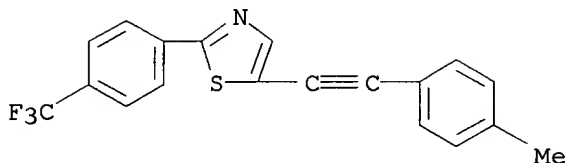
CN 2-Thiophenecarboxylic acid, 5-[5-(phenylethynyl)-2-thiazolyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 119539-82-1 CAPLUS

CN Thiazole, 5-[(4-methylphenyl)ethynyl]-2-[4-(trifluoromethyl)phenyl]- (9CI)

(CA INDEX NAME)



L37 ANSWER 39 OF 46 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1987:636598 CAPLUS

DOCUMENT NUMBER: 107:236598

TITLE: Palladium-catalyzed reactions of terminal acetylenes and olefins with halo-1,3-azoles

AUTHOR(S): Sakamoto, Takao; Nagata, Hideo; Kondo, Yoshinori; Shiraiwa, Masafumi; Yamanaka, Hiroshi

CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan

SOURCE: Chem. Pharm. Bull. (1987), 35(2), 823-8

CODEN: CPBTAL; ISSN: 0009-2363

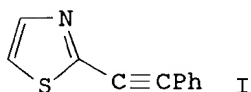
DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

OTHER SOURCE(S): CASREACT 107:236598

GRAPHIC IMAGE:



ABSTRACT:

The Pd-catalyzed reactions of 4-bromo- and 5-bromothiazoles, as well as 4-bromo- and 5-bromooxazoles with terminal acetylenes gave ethynyl derivs., e.g. I, in 43-89% yields, whereas the reactions of 2-bromothiazoles and iodo-N-methylimidazoles afforded the products in poor yields. The reaction of the halo-1,3-azoles with terminal olefins was also examd.

SUPPL. TERM: thiazole alkynyl alkenyl; oxazole alkynyl alkenyl; imidazole

alkynyl alkenyl; halothiazole alkynylation palladium catalyst; alkenylation haloazole palladium catalyst; heteroarom Heck arylation alkene alkyne

INDEX TERM: Alkenylation

Alkynylation

(of halooxazoles and halothiazoles)

INDEX TERM: Arylation

(Heck, of acetylenes and olefins with halooxazoles and

halothiazoles)

INDEX TERM: 7007-07-0 20662-93-5 28771-82-6 34259-99-9  
37067-95-1 57516-16-2 71759-87-0 71759-88-1  
ROLE: RCT (Reactant)  
(alkynylation and alkenylation of, in the presence of a  
palladium catalyst)

INDEX TERM: 3034-53-5 111600-83-0  
ROLE: RCT (Reactant)  
(alkynylation of, in the presence of a palladium  
catalyst)

INDEX TERM: 140-88-5, Ethyl acrylate 1066-54-2,  
(Trimethylsilyl)acetylene  
ROLE: RCT (Reactant)  
(arylation of, with bromothiazoles and -oxazoles,  
palladium catalyzed)

INDEX TERM: 536-74-3, Phenyl acetylene  
ROLE: RCT (Reactant)  
(arylation of, with halothiazoles and -oxazoles,  
palladium catalyzed)

INDEX TERM: 1826-12-6P 1826-17-1P 4072-63-3P **35070-01-0P**  
37570-94-8P 55384-94-6P 67879-31-6P 71759-92-7P  
83247-14-7P 108905-60-8P **111600-84-1P**  
111600-85-2P 111600-86-3P 111600-87-4P  
**111600-88-5P** 111600-89-6P 111600-90-9P  
111600-91-0P **111600-92-1P** 111600-93-2P  
111600-94-3P 111600-95-4P 111600-96-5P 111600-97-6P  
111600-98-7P 111600-99-8P 111601-00-4P 111601-01-5P  
111601-02-6P 111601-03-7P 111601-04-8P 111601-05-9P  
111601-06-0P 111601-07-1P 111601-08-2P 111601-09-3P  
111601-10-6P 111601-11-7P 111601-12-8P 111601-13-9P  
111601-14-0P **111601-15-1P** 111601-16-2P  
111601-17-3P 111620-41-8P  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

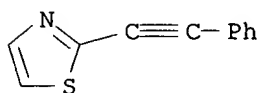
INDEX TERM: 107-13-1, Acrylonitrile, reactions  
ROLE: RCT (Reactant)  
(reaction of, with bromothiazoles and -oxazoles,  
palladium catalyzed)

INDEX TERM: 100-42-5, Styrene, reactions  
ROLE: RCT (Reactant)  
(reaction of, with halothiazoles and -oxazoles,  
palladium  
catalyzed)

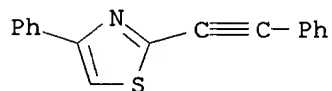
IT **35070-01-0P 111600-84-1P 111600-88-5P**  
**111600-92-1P 111601-15-1P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 35070-01-0 CAPLUS

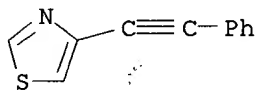
CN Thiazole, 2-(phenylethynyl)- (9CI) (CA INDEX NAME)



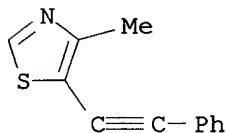
RN 111600-84-1 CAPLUS  
CN Thiazole, 4-phenyl-2-(phenylethynyl)- (9CI) (CA INDEX NAME)



RN 111600-88-5 CAPLUS  
CN Thiazole, 4-(phenylethynyl)- (9CI) (CA INDEX NAME)



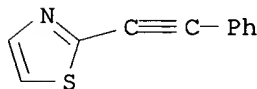
RN 111600-92-1 CAPLUS  
CN Thiazole, 4-methyl-5-(phenylethynyl)- (9CI) (CA INDEX NAME)



RN 111601-15-1 CAPLUS  
CN Thiazole, 2-(phenylethynyl)-, compd. with 2,4,6-trinitrophenol (1:1)  
(9CI) (CA INDEX NAME)

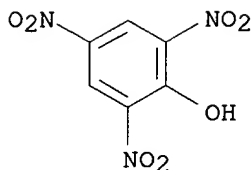
CM 1

CRN 35070-01-0  
CMF C11 H7 N S



CM 2

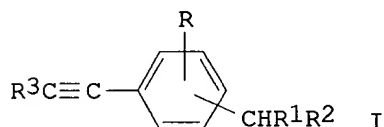
CRN 88-89-1  
CMF C6 H3 N3 O7



L37 ANSWER 40 OF 46 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1984:591680 CAPLUS  
 DOCUMENT NUMBER: 101:191680  
 TITLE: [(Heterocyclylethynyl)phenyl]acetic acid derivatives  
 PATENT ASSIGNEE(S): Mitsubishi Petrochemical Co., Ltd., Japan; Mitsubishi Yuka Pharmaceutical Co., Ltd.  
 SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 INT. PATENT CLASSIF.: C07D207-337; C07D209-18; C07D213-26; C07D213-55; C07D213-61; C07D277-22; C07D277-64; C07D307-54; C07D333-24; C07D333-28  
 ADDITIONAL: A61K031-34; A61K031-40; A61K031-425; A61K031-44  
 CLASSIFICATION: 27-8 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 1  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 59112963	A2	19840629	JP 1982-223259	19821220

GRAPHIC IMAGE:

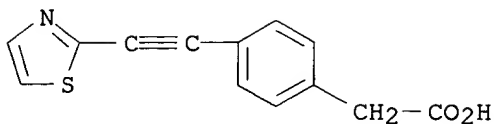


#### ABSTRACT:

The title compds. I [R = H, halo, CF<sub>3</sub>, alkyl, alkoxy; R<sub>1</sub> = H, Me, Et; R<sub>2</sub> = cyano, CO<sub>2</sub>H, alkoxy carbonyl, etc.; R<sub>3</sub> = (substituted) heterocyclyl], useful as antiinflammatory agents (carrageenan test in mice at 50 mg/kg p.o. given), were prepd. Thus, refluxing a mixt. of 650 mg CuC.tplbond.CC6H4CH<sub>2</sub>CO<sub>2</sub>Et-p, 654 mg 2-iodothiophene, and 30 mL pyridine for 3.5 h gave 420 mg I (R = H, CHR<sub>1</sub>R<sub>2</sub> = p-CH<sub>2</sub>CO<sub>2</sub>Et, R<sub>3</sub> = 2-thienyl).

SUPPL. TERM: antiinflammatory ethynylphenylacetate  
 INDEX TERM: Inflammation inhibitors and Antiarthritics  
 Inflammation inhibitors and Antiarthritics

((ethynylphenyl)acetic acid derivs.)  
 INDEX TERM: 4298-52-6 51551-95-2 92676-15-8 92708-45-7  
 ROLE: RCT (Reactant)  
 (ethynylation by, of (iodophenyl)acetonitrile derivs.)  
 INDEX TERM: 87356-22-7  
 ROLE: RCT (Reactant)  
 (ethynylation by, of haloheterocycle)  
 INDEX TERM: 87356-23-8 92676-21-6 92676-22-7  
 ROLE: RCT (Reactant)  
 (ethynylation by, of haloheterocycles)  
 INDEX TERM: 3437-95-4 5029-67-4  
 ROLE: RCT (Reactant)  
 (ethynylation of)  
 INDEX TERM: 87-32-1 3034-53-5 54829-48-0  
 ROLE: RCT (Reactant)  
 (ethynylation of, by (ethynylphenyl)acetate derivs.)  
 INDEX TERM: 92676-20-5  
 ROLE: RCT (Reactant)  
 (ethynylation of, by ethynylheterocycles)  
 INDEX TERM: 87356-21-6 92676-16-9 92676-17-0 92676-18-1  
 ROLE: RCT (Reactant)  
 (ethynylation of, with heterocyclethynylcopper)  
 INDEX TERM: 92676-19-2  
 ROLE: RCT (Reactant)  
 (hydrolysis of)  
 INDEX TERM: 92675-80-4P 92675-81-5P 92675-82-6P 92675-83-7P  
 92675-84-8P 92675-85-9P **92675-86-0P**  
 92675-87-1P 92675-88-2P 92675-89-3P 92675-90-6P  
 92675-91-7P 92675-92-8P 92675-93-9P 92675-94-0P  
 ROLE: BAC (Biological activity or effector, except  
 adverse);  
 SPN (Synthetic preparation); BIOL (Biological study); PREP  
 (Preparation)  
 (prepn. and antiinflammatory activity of)  
 INDEX TERM: 92675-95-1P 92675-96-2P 92675-97-3P 92675-98-4P  
 92675-99-5P **92676-00-1P** 92676-01-2P  
 92676-02-3P 92676-03-4P 92676-04-5P 92676-05-6P  
 92676-06-7P 92676-07-8P **92676-08-9P**  
 92676-09-0P **92676-10-3P** 92676-11-4P  
 92676-12-5P 92676-13-6P 92676-14-7P 92676-19-2P  
 92731-56-1P  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 IT **92675-86-0P**  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic  
 preparation); BIOL (Biological study); PREP (Preparation)  
 (prepn. and antiinflammatory activity of)  
 RN 92675-86-0 CAPLUS  
 CN Benzeneacetic acid, 4-(2-thiazolyethynyl)- (9CI) (CA INDEX NAME)

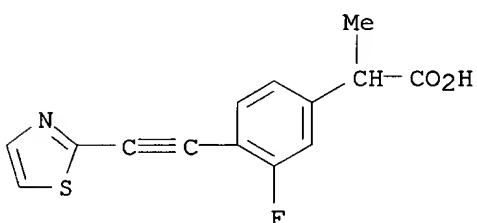


IT 92676-00-1P 92676-08-9P 92676-10-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

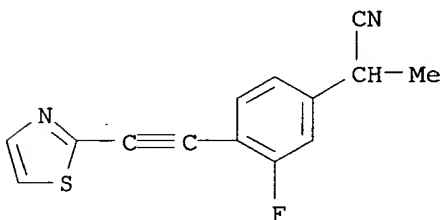
RN 92676-00-1 CAPLUS

CN Benzeneacetic acid, 3-fluoro-.alpha.-methyl-4-(2-thiazolylethynyl)- (9CI)  
(CA INDEX NAME)



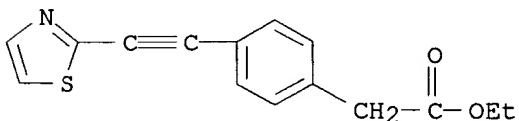
RN 92676-08-9 CAPLUS

CN Benzeneacetonitrile, 3-fluoro-.alpha.-methyl-4-(2-thiazolylethynyl)-  
(9CI)  
(CA INDEX NAME)



RN 92676-10-3 CAPLUS

CN Benzeneacetic acid, 4-(2-thiazolylethynyl)-, ethyl ester (9CI) (CA INDEX NAME)

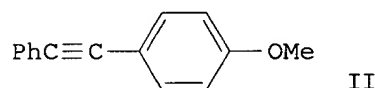




ACCESSION NUMBER: 1982:117583 CAPLUS  
 DOCUMENT NUMBER: 96:117583  
 TITLE: Soil disinfectant composition  
 PATENT ASSIGNEE(S): Kanesho Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 INT. PATENT CLASSIF.: A01N027-00; A01N029-00; A01N031-14; A01N043-06;  
 A01N043-40; A01N043-78  
 CLASSIFICATION: 5-2 (Agrochemical Bioregulators)  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56154401	A2	19811130	JP 1980-58501	19800501
JP 59028522	B4	19840713		

GRAPHIC IMAGE:

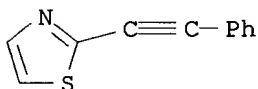


# ABSTRACT:

The compds. R1C.tplbond.CR2 (I; R1 and R2 = alkenyl, alkynyl, or arom.) are soil disinfectants. The synthesis of I is given. Thus, 200 ppm of II [7380-78-1] at 3 L/m3 soil controlled Pythium aphanidermatum on cucumber.

SUPPL. TERM: soil disinfectant compn  
 INDEX TERM: Bactericides, Disinfectants and Antiseptics  
 Bactericides, Disinfectants, and Antiseptics  
 (prepn. and activity of)  
 INDEX TERM: Fungicides and Fungistats  
 (soil disinfectant, prepn. and activity of)  
 INDEX TERM: 886-66-8P 1206-02-6P 1463-04-3P 3287-02-3P  
 3725-09-5P 4805-17-8P 5701-81-5P 7380-78-1P  
 13141-42-9P 13295-94-8P 13295-97-1P 13456-84-3P  
 13633-26-6P 23975-15-7P 28790-65-0P **35070-01-0P**  
 35133-77-8P 49836-17-1P 49836-18-2P 50559-45-0P  
 55110-61-7P 65406-81-7P 80221-12-1P 80221-14-3P  
 80221-15-4P 80221-19-8P 80221-20-1P 80746-49-2P  
 ROLE: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation);  
 BIOL  
 (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. and microbicidal activity of)  
 INDEX TERM: 109-89-7, reactions  
 ROLE: RCT (Reactant)  
 (reaction of, with bromochlorohexane, in soil disinfectant manuf.)  
 INDEX TERM: 536-74-3

ROLE: RCT (Reactant)  
 (reaction of, with bromopropane, in soil disinfectant  
 manuf.)  
 INDEX TERM: 696-62-8  
 ROLE: RCT (Reactant)  
 (reaction of, with phenylacetylene copper, in soil  
 disinfectant manuf.)  
 INDEX TERM: 106-94-5  
 ROLE: RCT (Reactant)  
 (reaction of, with phenylacetylene, in soil disinfectant  
 manuf.)  
 INDEX TERM: 1003-09-4  
 ROLE: RCT (Reactant)  
 (reaction of, with piperidine, in soil disinfectant  
 manuf.)  
 IT **35070-01-0P**  
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except  
 adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)  
 (prepn. and microbicidal activity of)  
 RN 35070-01-0 CAPLUS  
 CN Thiazole, 2-(phenylethynyl)- (9CI) (CA INDEX NAME)



L37 ANSWER 42 OF 46 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1982:16085 CAPLUS  
 DOCUMENT NUMBER: 96:16085  
 TITLE: Acetylene derivatives as nematocides  
 PATENT ASSIGNEE(S): Kanesho Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 INT. PATENT CLASSIF.: A01N027-00; A01N031-04; A01N031-08; A01N033-06;  
 A01N033-18; A01N035-04; A01N037-18; A01N037-34;  
 A01N043-06; A01N043-40; A01N043-78  
 CLASSIFICATION: 5-4 (Agrochemical Bioregulators)  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56123903	A2	19810929	JP 1980-27155	19800304
JP 59028521	B4	19840713		

ABSTRACT:

Acetylene derivs. are nematocides. The syntheses of such compds. are given.  
 Thus, 500 .mu.M MeO2CCH:CH.cntdot.C.tplbond.C.cntdot.CH:CHCO2Me [28813-55-0]  
 controlled *Pratylenchus coffeae* by 99.2% in 48 h.

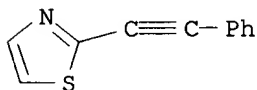
SUPPL. TERM: acetylene nematocide  
INDEX TERM: Nematocides  
(acetylenes)

INDEX TERM: 886-66-8 959-88-6 1206-02-6 1223-47-8 1463-04-3  
1820-42-4 1849-25-8 1849-26-9 1849-27-0 1942-30-9  
2735-14-0 2789-88-0 2789-89-1 3287-02-3 3725-09-5  
4805-17-8 5216-36-4 5293-78-7 5701-81-5 6775-17-3  
7380-78-1 13141-38-3 13141-40-7 13141-41-8  
13141-42-9 13141-44-1 13141-45-2 13295-94-8  
13295-97-1 13456-84-3 13633-26-6 22666-07-5  
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28813-55-0 29768-12-5 30405-77-7 35010-17-4  
**35070-01-0** 35133-77-8 41398-67-8 42296-34-4  
49836-17-1 49836-18-2 49836-19-3 49836-21-7  
50559-45-0 51118-06-0 54075-56-8 55110-61-7  
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61440-87-7 65406-81-7 74149-28-3 79135-69-6  
80220-64-0 80220-65-1 80220-66-2 80221-08-5  
80221-09-6 80221-10-9 80221-11-0 80221-12-1  
80221-13-2 80221-14-3 80221-15-4 80221-16-5  
80221-17-6 80221-18-7 80221-19-8 80221-20-1  
80221-21-2 80221-22-3 80221-23-4 80221-24-5  
80238-88-6  
ROLE: AGR (Agricultural use); BAC (Biological activity or  
effector, except adverse); BIOL (Biological study); USES  
(Uses)  
(nematocide)

INDEX TERM: 74-86-2D, derivs.  
ROLE: BIOL (Biological study)  
(nematocides)

IT **35070-01-0**  
RL: AGR (Agricultural use); BAC (Biological activity or effector, except  
adverse); BIOL (Biological study); USES (Uses)  
(nematocide)

RN 35070-01-0 CAPLUS  
CN Thiazole, 2-(phenylethynyl)- (9CI) (CA INDEX NAME)



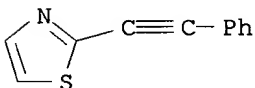
L37 ANSWER 43 OF 46 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 1972:59397 CAPLUS  
DOCUMENT NUMBER: 76:59397  
TITLE: Photochemical syntheses. V. Photoaddition of  
heterocyclic diarylacetylenes to naphthalene and  
1-methylnaphthalene  
AUTHOR(S): Teitei, T.; Collin, P. J.; Sasse, W. H. F.  
CORPORATE SOURCE: Div. Appl. Chem., CSIRO, North Ryde, Aust.  
SOURCE: Aust. J. Chem. (1972), 25(1), 171-82  
CODEN: AJCHAS  
DOCUMENT TYPE: Journal

LANGUAGE: English  
CLASSIFICATION: 27 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 24, 26  
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.

ABSTRACT:

Eight heterocyclic diarylacetylenes derived from pyridine, furan, thiophene, and thiazole were irradiated in the presence of naphthalene. Phenyl(4-pyridyl)-acetylene gave I and II, phenyl(3-pyridyl)acetylene gave III and IV, and phenyl(2-pyridyl)acetylene gave V and VI. From 1-methylnaphthalene and phenyl(3-pyridyl)acetylene the adducts VII and VIII were isolated and 2 adducts which formed by addn. to the unsubstituted ring were detected. From phenyl(2-thiazolyl)acetylene and naphthalene probably only one isomeric adduct IX was isolated. The methiodides of all the new adducts except IX were prepd. The structures proposed for these photo-adducts were based on their PMR, mass, and uv absorption spectra. Factors influencing the isomer distribution and overall yields were discussed.

SUPPL. TERM: photochem aryl acetylene naphthalene  
INDEX TERM: Cycloaddition reaction  
(photochem. of diarylacetylenes to naphthalene and methylnaphthalene)  
INDEX TERM: 90-12-0 91-20-3, reactions  
ROLE: RCT (Reactant)  
(photoaddn. reactions with diarylacetylenes)  
INDEX TERM: 35070-01-0P 35133-61-0P 35133-62-1P  
35133-63-2P 35133-64-3P 35133-65-4P 35133-66-5P  
35133-67-6P 35133-68-7P 35133-69-8P 35133-70-1P  
35133-72-3P 35133-73-4P 35133-74-5P 35133-75-6P  
35133-76-7P 35133-77-8P 35182-92-4P  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)  
IT 35070-01-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)  
RN 35070-01-0 CAPLUS  
CN Thiazole, 2-(phenylethynyl)- (9CI) (CA INDEX NAME)



L37 ANSWER 44 OF 46 USPATFULL

ACCESSION NUMBER: 2001:194516 USPATFULL  
TITLE: Preparation of substituted indoles  
INVENTOR(S): Henkelmann, Jochem, Mannheim, Germany, Federal  
Republic  
of  
Arndt, Jan-Dirk, Mannheim, Germany, Federal Republic  
of

NUMBER KIND DATE

PATENT INFORMATION:	US 2001037031	A1	20011101	
	US 6384235	B2	20020507	
APPLICATION INFO.:	US 2001-782310	A1	20010214	(9)

	NUMBER	DATE
PRIORITY INFORMATION:	DE 2000-10009000	20000225
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	Messrs. Keil & Weinkauff, 1101 Connecticut Ave., N. W., Washington, DC, 20036	
NUMBER OF CLAIMS:	10	
EXEMPLARY CLAIM:	1	
ABSTRACT:		

The present application describes a process for preparing compounds of the indole type of the formula ##STR1##

in which A is a hydrocarbon radical which, together with the carbons to which it is attached, forms a substituted or unsubstituted mono- or polycyclic aromatic system which may contain one or more heteroatoms from the group consisting of N, O and S, and

R.<sup>sup.1</sup>, R.<sup>sup.2</sup> independently of one another are H, a saturated, linear or branched aliphatic C.<sub>sub.1</sub>-C.<sub>sub.20</sub>-hydrocarbon radical, an unsaturated, linear or branched aliphatic C.<sub>sub.2</sub>-C.<sub>sub.20</sub>-hydrocarbon radical, a saturated or unsaturated, unsubstituted or alkyl-substituted cycloaliphatic C.<sub>sub.3</sub>-C.<sub>sub.20</sub>-hydrocarbon radical or an aromatic C.<sub>sub.5</sub>-C.<sub>sub.20</sub>-hydrocarbon radical, where these radicals may contain in their molecular skeleton one or more heteroatoms from the group consisting of the halogens, N, P, O, S, Si, Sn and B and may be substituted or unsubstituted,

by cyclization of alkynylaminoaromatics of the formula ##STR2##

in which R.<sup>sup.1</sup> and R.<sup>sup.2</sup> are as defined in formula (I) and R.<sup>sup.1</sup>, R.<sup>sup.2</sup> or A may be attached to an organic or inorganic carrier,

which comprises carrying out the reaction in a polar aprotic ion-solvating solvent in the presence of a suitable compound of Na, K, Rb or Cs.

Using this process, it is possible to prepare substituted indoles in a simple manner and in high yields.

[0001] The present invention relates to a process for preparing substituted indoles of the formula (I), in which substituted 2-alkynylanilines are cyclized in a polar aprotic solvent with the aid of a suitable alkali metal compound.

[0002] Simple, low-cost indole syntheses are of great general interest, since the indole structure is found in numerous natural products and in particular in pharmacologically active substances. To date, there are a number of principal

routes leading to the desired indole derivatives.

[0003] Intramolecular addition of amino groups to a carbon-carbon triple bond with formation of indole derivatives is a reaction known from the literature. The reaction can be catalyzed, for example, by palladium complexes. This is described, inter alia, in the publication by K. Utimoto et al. in Tetrahedron Letters 29 (1992), 3915 ff.

[0004] Other publications disclose the use of molybdenum(0) compounds in these cyclization reactions. This can be found in the publications by F. E. McDonald et al. in Tetrahedron Letters 38 (1997), 7687 ff. and in Chem. Eur. J. 5 (1999), 3103 ff.

[0005] In a variant described in a plurality of publications by S. Cacchi et al., for example in Tetrahedron Letters 33 (1992), 3915 ff., Synlett 1997, 1393 ff., Tetrahedron Letters 50 (1994), 437 ff., it is possible to use, instead of the alkynylanilines, the corresponding trifluoroacetamides, the catalysts used here again being palladium complexes.

[0006] The synthesis of substituted indoles is furthermore described by Yamanaka et al. in Heterocycles 24 (1986), 31/32. Here, alkynylcarbanilates are cyclized in the presence of Na ethoxylate, and the N-bonded C(O)O-alkyl unit is removed by hydrolysis. This cyclization reaction does not work if the starting material used is a 2-alkynylaniline.

[0007] However, in all of these reactions it is frequently necessary to heat the reaction mixture to relatively high temperatures, and frequently, long reaction times are additionally required to achieve acceptable yields. These harsh reaction conditions, which are generally required, strongly restrict, inter alia, the range of the various functionalities which can be present in the 2-alkynylanilines.

[0008] It is an object of the present invention to provide a process which allows a simple preparation of the substituted indoles, with good yields and using short reaction times and low reaction temperatures. The process should furthermore permit the synthesis of substituted indoles having a large number of different substituents.

[0009] We have found that this object is achieved by a process for preparing compounds of the indole type of the formula ##STR3##

[0010] in which A is a hydrocarbon radical which, together with the carbons to which it is attached, forms a substituted or unsubstituted mono- or polycyclic aromatic system which may contain one or more heteroatoms from the group consisting of N, O and S, and

[0011] R<sup>sup.1</sup>, R<sup>sup.2</sup> independently of one another are H, a saturated, linear or branched aliphatic C<sub>sub.1</sub>-C<sub>sub.20</sub>-hydrocarbon radical, an unsaturated, linear or branched aliphatic C<sub>sub.2</sub>-C<sub>sub.20</sub>-hydrocarbon radical, a saturated or unsaturated, unsubstituted or alkyl-substituted cycloaliphatic C<sub>sub.3</sub>-C<sub>sub.20</sub>-hydrocarbon radical or an aromatic C<sub>sub.5</sub>-C<sub>sub.20</sub>-

hydrocarbon radical, where these radicals may contain in their molecular skeleton one or more heteroatoms from the group consisting of the halogens, N, P, O, S, Si, Sn and B and may be substituted or unsubstituted,

[0012] by cyclization of alkynylaminoaromatics of the formula ##STR4##

[0013] in which R<sup>sup.1</sup> and R<sup>sup.2</sup> are as defined in formula (I) and R<sup>sup.1</sup>, R<sup>sup.2</sup> or A may be attached to an organic or inorganic carrier,

[0014] which comprises carrying out the reaction in a polar aprotic ion-solvating solvent in the presence of a suitable compound of Na, K, Rb or Cs.

[0015] We have found that the process according to the invention permits access to a large number of compounds of the indole type of a range which has not been possible with the processes of the prior art. By using the alkali metal compounds which are employed in the process according to the invention, it is possible to prepare indole derivatives which may have virtually any customary substituents R<sup>sup.1</sup>, R<sup>sup.2</sup>. In the individual case, the accessibility of certain substituted indole derivatives depends on the influence of certain parameters. These are, for example, steric interactions between the individual substituents present, and possibly also the aromatic system of the indole derivative. The range of the different substituents R<sup>sup.1</sup> and R<sup>sup.2</sup> and of the substituents which may be present on the aromatic system of the formula (I) is enormously wide and comprises virtually all compound classes and functional groups which are included in the definition given above.

[0016] In a preferred embodiment of the present invention, the substituents R<sup>sup.1</sup> and R<sup>sup.2</sup> independently of one another are selected from the group consisting of H, linear and branched C<sub>sub.1</sub>-C<sub>sub.12</sub>-alkyl groups, linear and branched C<sub>sub.2</sub>-C<sub>sub.12</sub>-alkenyl groups, C<sub>sub.3</sub>-C<sub>sub.8</sub>-cycloalkyl groups, C<sub>sub.3</sub>-C<sub>sub.8</sub>-cycloalkenyl groups, C<sub>sub.5</sub>- and C<sub>sub.6</sub>-heterocycles having one or more ring atoms selected from the group consisting of N, O and S and mono- or bicyclic aromatics having one or more ring atoms selected from the group consisting of N, O and S.

[0017] Both in the preferred and the not preferred embodiments, the substituents R<sup>sup.1</sup> and R<sup>sup.2</sup> may have one or more substituents in their molecular skeleton.

[0018] Examples of preferred substituents are amino and nitro groups, halogens, hydroxyl and ether groups, thiol groups, thioether groups, amide and ester groups, sulfaryl groups and sulfoxide groups.

[0019] The aromatic system in the compounds of the formula (I) can be a mono- or polycyclic aromatic which comprises exclusively carbon and hydrogen or which may have one or more heteroatoms selected from the group consisting of N, O and S.

[0020] The aromatic system is preferably a mono- or bicyclic aromatic. More preferably, the aromatic system is a C.sub.5-heterocycle or a benzene or naphthalene derivative which may contain one or more of the heteroatoms N, O and S mentioned, examples being benzene and naphthalene, aza-, diaza- and triazabenzene, aza-, diaza- and triazanaphthalene, thiophene and furan.

[0021] In the most preferred embodiment of the present invention, the aromatic system in the formula (I) is selected from the group consisting of benzene, naphthalene, pyridine, pyrazine, pyrimidine, quinoline, thiophene and furan.

[0022] Both in the preferred and the not preferred embodiments, the aromatic system may have one or more substituents which, similarly to the substituents R.sup.1 and R.sup.2, may vary extremely. Non-limiting examples of such substituents are alkanes and alkenes which are either unsubstituted or may carry customary substituents, for example halogens, amines, nitro groups, ether and hydroxyl groups or thiol- and thioether groups. Further examples of substituents on the aromatic system are amino and nitro groups, halogens, hydroxyl and ether groups, thiol groups, sulfaryl groups, sulfoxide groups, thioether groups, amide and ester groups.

[0023] In one embodiment of the present invention, the synthesis of the indole derivatives (I) can be carried out by attaching the alkynylaminoaromatic (II) used as starting material to an organic or inorganic carrier and immobilizing it. These carriers are known to the person skilled in the art and correspond to the customary carrier materials used, for example, for solid-phase peptide synthesis or for fixing transition metal catalyst systems. Examples are Merrifield resin, 4-(2',4'-dimethoxyphenyl-Fmoc-aminomethyl)-phenoxyacetamidonorleucyl- methylbenzhydrylamino-(divinylbenzene-crosslinked polystyrene) resin, also known under the name Rink-MBHA resin, which is generally used after deprotection by removal of the 9-fluorenylmethoxycarbonyl-(Fmoc) group, and the carrier resin which is commercially available under the name trityl chloride resin, if appropriate after appropriate modification.

[0024] These carriers are either bonded to the aromatic system of the starting materials (II), or the substituent R.sup.1 is attached to the carrier. If appropriate, the carrier may have suitable spacer groups which are attached to the starting material. Following the synthesis of the corresponding indole compound, the bond between the carrier and the target molecule is broken in a customary manner known to the person skilled in the art, for example by cleaving the bond between carrier and spacer group using trifluoroacetamide.

[0025] A further embodiment of the present invention allows the synthesis of compounds (I) in which the aromatic system, which is fused with the pyrroline unit, forming a bicyclic indole unit, is fused with a further pyrroline unit, forming a tricyclic bifunctional indole. To this end, the starting material (II) used is a compound which does not only have one acetylene function and one amino function in a vicinal position, but in each case two of these functions.

[0026] The synthesis element according to the invention can also be widened such that the resulting indole does not only contain 2 pyrroline units, but 3



or even more of these units. To this end, a starting material (II) is used which contains 3 or even more vicinal acetylene and amino functions.

[0027] The synthesis according to the invention is carried out using a suitable compound of Na, K, Rb or Cs, which is employed in combination with a polar aprotic solvent having ion-solvating properties. By using these solvents, it is possible to increase the electrophilicity of the ions of the metals mentioned such that the cyclization according to the invention can be carried out under mild conditions.

[0028] These polar aprotic ion-solvating solvents are known to the person skilled in the art, examples being N-methylpyrrolidone (NMP), N-butylpyrrolidone (NBP), dimethyl sulfoxide (DMSO), sulfolane (tetrahydrothiophene 1,1-dioxide), dimethylformamide (DMF), tetrahydrofuran (THF), ethers, hexamethylphosphoric triamide (HMPT) and N,N'-dimethylpropyleneurea.

[0029] Examples of suitable ethers are ethers which can be obtained from ethylene oxide and/or propylene oxide. This can be ethylene glycol and propylene glycol ethers, oligo- or polyethylene glycol, oligo- and polypropylene glycol and ethylene glycol/propylene glycol copolymers or block copolymers, such as, for example, the compounds known under the names glyme, diglyme, triglyme or the names Pluronic.RTM. and Pluriol.RTM. (from BASF AG). It is also possible to use ethers which are prepared by condensing ethylene oxide and/or propylene oxide with polyvalent amines, for example the products available under the names Tetronic.RTM. and Lutensol.RTM. (in each case from BASF AG).

[0030] It is also possible to use the respective ethers, for example the methyl ethers, of all of the abovementioned ethylene glycol and propylene glycol ethers, which, for example in the case of Pluronic.RTM., Pluriol.RTM. and Tetronic.RTM., may still have free terminal hydroxyl groups. Suitable ethers are also crown ethers and cryptands.

[0031] These solvents can be used on their own, as a mixture or as additive to other solvents. They have to be added in an amount which is sufficient to achieve the desired ion solvation and thus the required reactivity.

[0032] The compounds of Na, K, Rb and Cs which are employed are those which dissociate well in the solvents mentioned and whose ions are sufficiently solvated by these solvents. Examples of suitable compounds of the alkali metals quoted are hydroxides, hydrides, alkoxides, amides and aminopropylamides.

[0033] Particularly suitable compounds are hydroxides and alkoxides.

[0034] Among the abovementioned metals Na, K, Rb and Cs, the best reactivities are obtained when K and Cs are used, and their use is preferred. The alkali metal compounds used according to the invention can be employed in stoichiometric or superstoichiometric amounts, but also in catalytic amounts. The minimum amount of alkali metal compounds is about 5 mol %; however, it is also possible to use amounts of up to 250 mol %, based on the substrate. The

reaction temperatures required for the process according to the invention are about <100.degree. C. The process according to the invention is preferably carried out at temperatures of about 20-60.degree. C., most preferably of about

20-40.degree. C. The reaction times are from about 2 to 20 hours, preferably from 2 to 8 hours. The starting materials (II) are obtained by the Sonogashira reaction (see K. Sonogashira et al., Synthesis 1980, 627 ff., K. Sakamoto, Synthesis 1983, 312 ff., G. C. Fu et al., Angew. Chem. Int. Ed. Engl. 38 (1999), 2411 ff.) from the corresponding 2-iodo- or 2-bromoanilines by reaction

with 1 -alkynes. If the process according to the invention is carried out on a carrier, in solid phase, the corresponding iodo- or bromoaniline is, prior to the Sonogashira coupling, fixed to the carrier using methods known to the person skilled in the art. The invention is now illustrated by the examples below.

#### EXAMPLE 1

[0035] Synthesis of 2-phenylindole using different alkali metal compounds

[0036] A solution of 1.05 mmol of the alkali metal compound in question was dissolved or suspended under argon in 4 ml of NMP. 97 mg (0.5 mmol) of 2-phenylethynylaniline in 1 ml of NMP were then added. The solution was then stirred vigorously at the temperatures given in Table 1, for the stated reaction times. 1 ml of water and 50 ml of dichloromethane were then added, and the resulting solution was washed with a saturated NaCl solution. The solution was dried over MgSO<sub>4</sub>, the residue was filtered off, the solution was concentrated under reduced pressure and the resulting residue was then purified chromatographically on a silica gel column using a CH<sub>2</sub>Cl<sub>2</sub>/pentane mixture. Removal of the solvent gave the pure product.

[0037] The results are shown in Table 1. The stated yields are based on analytically pure end product.

TABLE 1

Experiment	Base	Temp. [.degree. C.]	Time [h]	Yield [%]
A	NaH	60	8	>5
B	NaOEt	80	15	66
C	KOt-Bu	25	4	79
D	KH	25	5	72
E	CsOH	90	5	68
F	CsOt-Bu	25	5	71

#### EXAMPLE 2

[0038] Synthesis of different indole and azaindole derivatives

[0039] Method A

[0040] Under argon, 0.5 mmol of the starting material in question is added to a

stirred solution of 42 mg (1.05 mmol) of KH in 4 ml of NMP. After 3 to -12 hours at room temperature, the reaction solution was worked up as in Example 1.

The results are shown in Table 2.

[0041] Method B

[0042] The reaction was carried out as described under A, using the alkali metal compound KOt-Bu. The reaction time was 4 hours at room temperature. Work-up, too, was carried out as described in Example 1. The results are also shown in Table 2.

TABLE 2

Ex- Yield periment Method	Aniline used [%]	Indole derivative obtained
1	##STR5##	##STR6##
A(B)	1a:R = Ph 72(79)	2a:R = Ph
2	1b:R = Bu	2b:R = Bu
A(B)	76(78)	
3	1c:R = 1-cyclo-	2c:R =
A	67 hexenyl	1-cyclohexenyl
4	1d:R = H	2d:R = H
B	62	
5	1e:R = (CH.sub.2).sub.2OH (CH.sub.2).sub.2OH A	2e:R =
6	1f:R = CH(OEt).sub.2	2f:R = CH(Oet).sub.2
B	81	
7	1g:R2-thienyl	2g:R = 2-thienyl
A	70	
8	1h:R = 2-thiazole	2h:R = 2-thiazole
A	61	
9	1i:R3-chloropropyl	2i:R = 3-cyclo-
A	75	propyl
10	1j:R =	2j:R = 2-amino-
A	82 2-aminophenyl	phenyl
11	##STR7##	##STR8##
A	80	
12	##STR9##	##STR10##
B	77	
13	##STR11##	##STR12##
A	72	

14	##STR13##	##STR14##
A	74	
15	##STR15##	##STR16##
B	78	
16	##STR17##	##STR18##
B	61.sup.a)	
17	##STR19##	##STR20##
B	80.sup.b)	
18	##STR21##	##STR22##
B	90.sup.b)	

.sup.a) 60.degree. C./5 h  
 .sup.b) 80.degree. C./6 h

### EXAMPLE 3

[0043] Solid-phase synthesis of substituted indoles ##STR23##

[0044] a) preparation of starting material 3

[0045] Deprotected Rink-MBHA resin (2 g; 0.64 mmol/g, obtainable by reaction of Rink-MBHA resin with piperidine, was, in a shaker glass fitted with septum and filled with argon, swollen for about 10 min in dichloromethane (15 ml) and then admixed with 4-iodobenzoic acid (478 mg; 1.92 mmol) and N,N'-diisopropylcarbodiimide (DIC) (240 mg; 1.92 mmol). The suspension was shaken at room temperature for 20 h. The polymer was filtered and washed alternately with dichloromethane, methanol, THF and DMF (in each case about 15 ml). The washing procedure was repeated three times. The polymer was then washed four times with dichloromethane (in each case about 15 ml) and dried at 55.degree. C. for about 16 h.

[0046] b) The resulting product was then subjected to two successive Sonogashira couplings, the cyclization according to the invention and cleavage from the polymer resin.

[0047] To this end, in the first coupling, polymer-bound 4-iodobenzamide (500 mg; 0.25 mmol), Pd(PPh.sub.3).sub.2Cl.sub.2 (17.4 mg; 0.025 mmol) and CuI (11.8 mg; 0.062 mmol) were initially charged in a Schlenk tube, fitted with septum and filled with argon, and swollen in toluene (5 ml) for about 10 min. Diethylamine (5 ml) was then added, the mixture was cooled to 0.degree. C. and trimethylsilylacetylene (245 mg; 2.5 mmol) was added. The mixture was stirred at room temperature for 12 h and the polymer was then filtered and washed with DMF, methanol and THF (in each case about 10 ml). The washing procedure was repeated four times. The polymer was then washed four times with

dichloromethane (in each case about 10 ml) and then admixed with TBAF (5 ml; 0.25 M in THF) and shaken for about 15 min. The resin was washed as described above and dried at 55.degree. C. for about 16 h.

[0048] The second coupling was carried out like the first coupling, including washing procedure and drying.

[0049] The following amounts were used:

[0050] Resin-bonded 4-ethynylbenzamide (400 mg; 0.22 mmol); Pd(PPh.sub.3).sub.2Cl.sub.2 (15.4 mg; 0.022 mmol); CuI (10.5 mg; 0.055 mmol); toluene (4 ml); diethylamine (4 ml); 2-iodoaniline (450 mg; 2.2 mmol).

[0051] The resulting resin-bound amino-substituted diphenylacetylene can also be obtained in one step from the resin-bound 4-iodobenzamide and 2-trimethylsilylethynylaniline. This process is carried out exactly like the first coupling, including washing procedure and drying, the only modification being that here the terminal alkyne is generated beforehand by deprotection with tetrabutylammonium fluoride (TBAF) in THF and added after substantial removal of the solvent under high vacuum.

[0052] The following amounts were used:

[0053] Resin-bound 4-iodobenzamide (500 mg; 0.25 mmol); Pd(PPh.sub.3).sub.2Cl.sub.2 (17.5 mg; 0.025 mmol); CuI (11.9 mg; 0.063 mmol); toluene (5 ml); diethylamine (5 ml); 2-trimethylsilylethynylaniline (475 mg; 2.5 mmol); TBAF (11.0 ml, 2.75 mmol).

[0054] The resulting intermediate was then cyclized to give the indole, as follows:

[0055] The polymer-bound starting material (200 mg; 0.09 mmol) was initially charged in a Schlenk tube, fitted with septum and filled with argon, and swollen in NMP (4 ml) for about 5 min. The mixture was then cooled to 0.degree.

C., and a solution of K<sup>+</sup>tBu<sup>-</sup> (150 mg; 1.35 mmol) in NMP (12 ml) was added dropwise. The mixture was then stirred at room temperature for 24 h, and the resin was filtered and washed with dichloromethane, THF, methanol, DMF (in each case about 5 ml). The washing procedure was repeated about ten to twelve times.

The polymer was then washed four times with dichloromethane (in each case about 5 ml) and dried at 55.degree. C. for about 16 h.

[0056] The resulting resin was then cleaved using TFA/dichloromethane 1:1.  
##STR24##

[0057] The Sonogashira coupling was carried out as described above under A, but at 80.degree. C. over the course of 18 h, and the starting material used was resin-bound 2-bromo-4-methylaniline. 50 mol % of CuI were used. The reaction with K<sup>+</sup>tBu<sup>-</sup> was then carried out by method A, as was the cleavage of the resin.

What is claimed is:

1. A process for preparing compounds of the indole type of the formula ##STR25## in which A is a hydrocarbon radical which, together with the carbons to which it is attached, forms a substituted or unsubstituted mono- or polycyclic aromatic system which may contain one or more heteroatoms from the group consisting of N, O and S, and R<sup>sup.1</sup>, R<sup>sup.2</sup> independently of one another are H, a saturated, linear or branched aliphatic C<sub>sub.1</sub>-C<sub>sub.20</sub>-hydrocarbon radical, an unsaturated, linear or branched aliphatic C<sub>sub.2</sub>-C<sub>sub.20</sub>-hydrocarbon radical, a saturated or unsaturated, unsubstituted

or alkyl-substituted cycloaliphatic C<sub>sub.3</sub>-C<sub>sub.20</sub>-hydrocarbon radical or an aromatic C<sub>sub.5</sub>-C<sub>sub.20</sub>-hydrocarbon radical, where these radicals may contain

in their molecular skeleton one or more heteroatoms from the group consisting of the halogens, N, P, O, S, Si, Sn and B and may be substituted or unsubstituted, by cyclization of alkynylaminoaromatics of the formula ##STR26## in which R<sup>sup.1</sup> and R<sup>sup.2</sup> are as defined in formula (I) and R<sup>sup.1</sup>, R<sup>sup.2</sup> or A may be attached to an organic or inorganic carrier, which comprises carrying out the reaction in a polar aprotic ion-solvating solvent in the presence of a suitable compound of Na, K, Rb or Cs, preferably K or Cs.

2. A process as claimed in claim 1, wherein the substituents R<sup>sup.1</sup> and R<sup>sup.2</sup> independently of one another are selected from the group consisting of H, linear and branched C<sub>sub.1</sub>-C<sub>sub.12</sub>-alkyl groups, linear and branched C<sub>sub.2</sub>-C<sub>sub.12</sub>-alkenyl groups, C<sub>sub.3</sub>-C<sub>sub.8</sub>-cycloalkyl groups, C<sub>sub.3</sub>-C<sub>sub.8</sub>-cycloalkenyl groups, C<sub>sub.5</sub>- and C<sub>sub.6</sub>-heterocycles having one or more ring atoms selected from the group consisting of N, O and S and mono- or bicyclic aromatics having one or more ring atoms selected from the group consisting of N, O and S.

3. A process as claimed in claim 1, wherein the hydrocarbon groups defined for R<sup>sup.1</sup> and R<sup>sup.2</sup> carry one or more substituents selected from the group consisting of amino and nitro groups, halogens, hydroxyl and ether groups, thiol groups, thioether groups, amide and ester groups, sulfaryl groups and sulfoxide groups.

4. A process as claimed in claim 1, wherein a hydride, hydroxide, alkoxide, amide or aminopropylamide of Na, K, Rb or Cs is used.

5. A process as claimed in claim 1, wherein the solvent used is N-methylpyrrolidone, N-butylpyrrolidone, dimethyl sulfoxide, sulfolane, dimethylformamide, tetrahydrofuran, hexamethylphosphoric triamide, N,N'-dimethylpropyleneurea or an ether, in particular an ether prepared from ethylene oxide and/or propylene oxide or from ethylene oxide and propylene oxide and a polyvalent amine, or a mixture of these solvents.

6. A process as claimed in claim 1, wherein the aromatic system in the compound of the formula (I) is a substituted or unsubstituted mono- or bicyclic aromatic, preferably a substituted or unsubstituted aromatic selected from the group consisting of C<sub>sub.5</sub>-heterocycles, benzene and naphthalene derivatives, most preferably from the group consisting of benzene, naphthalene, pyridine, pyrazine, pyrimidine, quinoline, thiophene and furan.

7. A process as claimed in claim 1, wherein the alkali metal compound is employed in an amount of from 5 mol % to 150 mol %, based on the substrate.

8. A process as claimed in claim 1, wherein the process is carried out at temperatures <100.degree. C., preferably at 20-60.degree. C., most preferably at 20-40.degree. C.

9. A process as claimed in claim 1, wherein the reaction time is from 2 to 20 hours, preferably from 2 to 8 hours.

10. A process as claimed in claim 1, wherein the alkynylaminoaromatic (II) used as starting material is attached to an organic or inorganic carrier, preferably selected from the group consisting of Merrifield resin, rink-MHBA resin and trityl chloride resin, if appropriate after appropriate modification, and immobilized, and the bond between carrier material and target molecule is broken in a manner known per se when the synthesis has ended.

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SECONDARY: 548/427.000

CURRENT U.S. PATENT CLASSIF.:

MAIN: 548/494.000

SECONDARY: 548/495.000

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MAIN: C07D209-56

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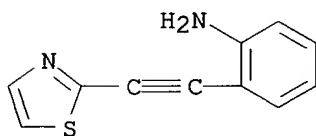
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 288254-66-0

(prepn. of indole-type compds. by cyclization of alkynylanilines or .alpha.-amino-.beta.-alkynylheterocycles in presence of alkali metal compd. in polar aprotic solvent)

RN 288254-66-0 USPATFULL

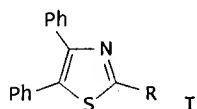
CN Benzenamine, 2-(2-thiazolylethynyl)- (9CI) (CA INDEX NAME)



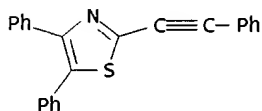
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L54 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1990:515155 HCAPLUS  
 DN 113:115155  
 TI Synthesis of 4,5-diarylthiazole derivatives as blood platelet aggregation inhibitors  
 AU Konno, Shoetsu; Amano, Masaki; Sagi, Mataichi; Yamanaka, Hiroshi  
 CS Pharm. Inst., Tohoku Univ., Sendai, 980, Japan  
 SO Yakugaku Zasshi (1990), 110(2), 105-14  
 CODEN: YKKZAJ; ISSN: 0031-6903  
 DT Journal  
 LA Japanese  
 OS CASREACT 113:115155  
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AB A no. of 2-substituted 4,5-diphenylthiazoles I [R = OMe, OEt, OCHMe2, OBU, OCHMeEt, OPh, NHNH2, NHBu, piperidino, 4-methylpiperazino, CH2COPh, C(CN)CO2Et, C(CO2Et)2, CH2CO2Me] were synthesized by the nucleophilic substitution of I (R = SO2Me) with various sodium alkoxides, amines, and carbanions of active methylene compds. 2-Ethynyl-4,5-diphenylthiazoles I (R = C.tplbond.CR1; R1 = Me, Ph, Bu, SiMe3) were synthesized by palladium cross-coupling reaction of I (R = iodo) with monosubstituted acetylene. I (R = alkoxy, 4-methylpiperazino) have potent inhibitory activity.  
 IT 129206-42-4P, 4,5-Diphenyl-2-phenylethynylthiazole  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of, as blood platelet aggregation inhibitor)  
 RN 129206-42-4 HCAPLUS  
 CN Thiazole, 4,5-diphenyl-2-(phenylethynyl)- (9CI) (CA INDEX NAME)





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L35 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2001 ACS

AN 1997:416781 HCAPLUS  
 DN 127:34399  
 TI Preparation of thiamorphinans with neuroprotective activity  
 IN Lemaire, Simon  
 PA Biochem Pharma Inc., Can.; Lemaire, Simon  
 SO PCT Int. Appl., 43 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9716183	A1	19970509	WO 1996-CA728	19961030
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG				
CA 2232355	AA	19970509	CA 1996-2232355	19961030
AU 9672745	A1	19970522	AU 1996-72745	19961030
AU 701346	B2	19990128		
EP 858333	A1	19980819	EP 1996-934278	19961030
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1205633	A	19990120	CN 1996-199227	19961030
JP 11514383	T2	19991207	JP 1996-516948	19961030
NO 9801939	A	19980429	NO 1998-1939	19980429
US 5955493	A	19990921	US 1998-66453	19980430
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WO 1996-CA728		19961030		
OS MARPAT 127:34399				
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The thiamorphinan derivs. I (R = H, halo, OH, amino, CO<sub>2</sub>H, alkoxycarbonyl, acyl, acyloxy, alkoxy, mercapto, alkylthio, carbocyclic or heterocyclic ring; X = S, alkylthionium, SO, SO<sub>2</sub>; m = 0-3, n = 0-2) were prepd. as neuroprotectives against excitatory amino acid (EAA) cytotoxicity. In particular, morphinan derivs. of the invention act as antagonists at the ionotropic NMDA (N-methyl-(D)-aspartic acid) receptor and are useful as protective agents against peripheral and central nervous system NMDA-receptor mediated toxicity and convulsions. Thus, the phenanthrene deriv. II, prepd. in 8 steps from the tetrolone III via spiro deriv. IV, was cyclized to the deazathiamorphinan followed by demethylation and allylation to give the thionium deazathiamorphinan V. The CD<sub>50</sub> of V for inhibition of NMDA induced convulsion was 0.07 nmol/mouse.

=> d bib abs hitstr 135 2

L35 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1993:485793 HCAPLUS  
 DN 119:85793  
 TI Heterocyclic modulators of the NMDA receptor  
 AU Pellicciari, Roberto; Natalini, Benedetto; Costantino, Gabriele; Garzon, Aaron; Luneia, Roberto; Mahmoud, Mahmoud R.; Marinozzi, Maura; Roberti, Marinella; Rosato, Giovanni C.; Shiba, Sayed A.  
 CS Ist. Chim. Farm. Tec. Farm., Univ. Perugia, Perugia, Italy  
 SO Farmaco (1993), 48(2), 151-7  
 CODEN: FRMCE8  
 DT Journal  
 LA English  
 AB The design of new heterocyclic derivs. as modulatory agents at excitatory amino acid receptors is described. In particular, the potent and selective activity at the NMDA receptor of trans-4-hydroxy-pipecolic acid-4-sulfate, as well as the neuroprotective properties of substituted thiokynurenates, a new class of competitive antagonists at the glycine site of the NMDA receptor complex, are reported.

=&gt; d bib abs hitstr 134 1

**L34 ANSWER 1 OF 3 HCAPLUS** COPYRIGHT 2001 ACS

AN 1999:184245 HCAPLUS

DN 130:223301

TI Preparation of 6,7-asymmetrically disubstituted quinoxalinecarboxylic acid derivatives and addition salts thereof as selective antagonists of AMPA receptor

IN Takano, Yasuo; Shiga, Futoshi; Takadoi, Masanori; Uchiki, Hideharu; Asano, Jun; Anraku, Tsuyoshi; Fukuchi, Kazunori; Uda, Junichiro; Ando, Naoki

PA Kyorin Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 293 pp.

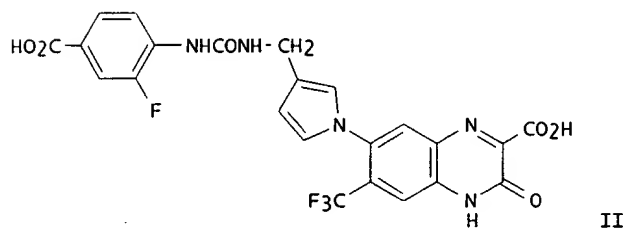
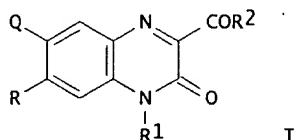
CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9911632	A1	19990311	WO 1998-JP3832	19980828
	W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	JP 2000080085	A2	20000321	JP 1998-291295	19980826
	AU 9888864	A1	19990322	AU 1998-88864	19980828
	EP 1020453	A1	20000719	EP 1998-940594	19980828
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
	BR 9811739	A	20000919	BR 1998-11739	19980828
	NO 2000001046	A	20000502	NO 2000-1046	20000301
PRAI	JP 1997-251313		19970901		
	JP 1998-190108		19980706		
	JP 1998-190109		19980706		
	WO 1998-JP3832		19980828		
OS	MARPAT 130:223301				
GI					



AB Claimed and prepd. are the disubstituted quinoxalinecarboxylic acid derivs. represented by formula [I; wherein Q is halogeno, optionally halogenated lower alkyl, Ar-P- (wherein Ar is Ph optionally substituted with one or more substituting groups, or naphthyl; and P is lower alkylene, lower alkenylene, lower alkynylene, oxygen or sulfur), etc.; R is nitro, trifluoromethyl, optionally substituted amino or a group of general formula NS(O)NR1OR11 (wherein R10 and R11 represent H, optionally halo-substituted alkyl, cycloalkyl, aralkyl, Ph, or optionally fused heterocyclyl; or NR1OR11 forms a ring optionally contg. 1 or 2 heteroatoms; n is 1 or 2); R1 is aralkyl, Ph, naphthyl, a 5- or

SEARCHED BY SUSAN HANLEY 305-4053

6-membered heterocycle or a fused ring thereof (which may have one or more substituting groups on the arom. ring or the heterocycle), hydrogen, optionally halogenated lower alkyl or cycloalkyl; and R2 is hydroxyl, lower alkoxy or a group of general formula NR8R9 (wherein R8 and R9 are aralkyl, Ph, optionally fused heterocyclyl, H, optionally halo-substituted alkyl, or cycloalkyl; or NR8R9 forms a ring optionally contg. 1 or 2 heteroatoms)]. Also claimed are antagonists of excitatory amino acid receptors comprising as the active ingredient 6,7-asym. disubstituted quinoxalinecarboxylic acid derivs. or addn. salts thereof, particularly compds. exhibiting antagonism against AMPA receptors (non-NMDA receptor); and processes for the prepn. of both. They are useful for the treatment of brain nerve cell disorders related to nerve cell death, so called excitotoxicity caused by excessive excitation of glutamic acid receptors. Thus, addn. reaction of Et 7-(3-(aminomethyl)pyrrol-1-yl)-3-oxo-1,2,3,4-tetrahydro-6-(trifluoromethyl)quinoxaline-2-carboxylate hydrochloride with Et 3-fluoro-4-isocyanatobenzoate followed by 2,3-dichloro-5,6-dicyanoquinone oxidn. and sapon. gave the title compd. (II). II in vitro showed the binding affinity to a synaptosome prepn. from rat cerebral cortex with Ki of 11.8 nM.

IT 221165-51-1P 221165-82-8P 221166-19-4P

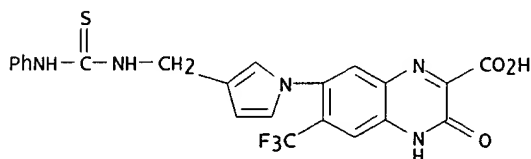
221166-69-4P 221166-70-7P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of asym. disubstituted quinoxalinecarboxylic acid derivs. as selective antagonists of AMPA receptor for treatment of brain nerve cell disorders)

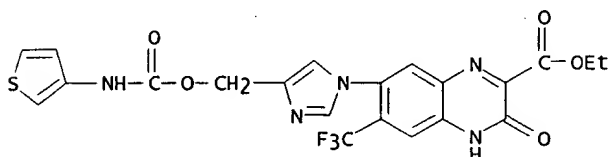
RN 221165-51-1 HCAPLUS

CN 2-Quinoxalinecarboxylic acid, 3,4-dihydro-3-oxo-7-[3-[[[(phenylamino)thioxomethyl]amino]methyl]-1H-pyrrol-1-yl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



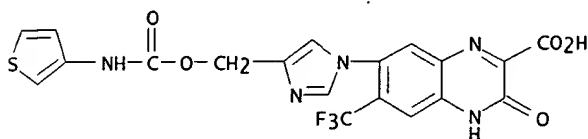
RN 221165-82-8 HCAPLUS

CN 2-Quinoxalinecarboxylic acid, 3,4-dihydro-3-oxo-7-[4-[[[(3-thienylamino)carbonyloxy]methyl]-1H-imidazol-1-yl]-6-(trifluoromethyl)-ethyl ester (9CI) (CA INDEX NAME)



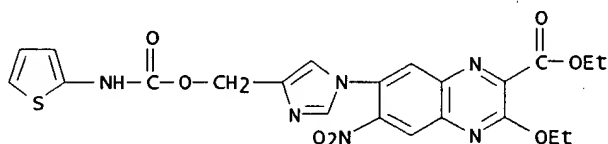
RN 221166-19-4 HCAPLUS

CN 2-Quinoxalinecarboxylic acid, 3,4-dihydro-3-oxo-7-[4-[[[(3-thienylamino)carbonyloxy]methyl]-1H-imidazol-1-yl]-6-(trifluoromethyl)-ethyl ester (9CI) (CA INDEX NAME)

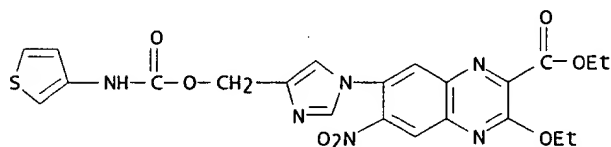


RN 221166-69-4 HCAPLUS

CN 2-Quinoxalinecarboxylic acid, 3-ethoxy-6-nitro-7-[4-[[[(2-thienylamino)carbonyl]oxy]methyl]-1H-imidazol-1-yl]-, ethyl ester (9CI)  
(CA INDEX NAME)

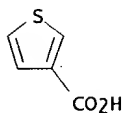


RN 221166-70-7 HCAPLUS  
CN 2-Quinoxalinecarboxylic acid, 3-ethoxy-6-nitro-7-[4-[[[(3-thienylamino)carbonyl]oxy]methyl]-1H-imidazol-1-yl]-, ethyl ester (9CI)  
(CA INDEX NAME)



IT 88-13-1, Thiophene-3-carboxylic acid  
RL: RCT (Reactant)  
(prepn. of asym. disubstituted quinoxalinecarboxylic acid derivs. as selective antagonists of AMPA receptor for treatment of brain nerve cell disorders)

RN 88-13-1 HCAPLUS  
CN 3-Thiophenecarboxylic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



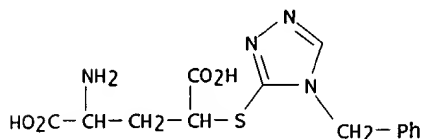
RE.CNT 17  
RE

- (1) Birch, P; European Journal of Pharmacology 1989, V163(1), P127 HCAPLUS
  - (2) Eli Lilly And Co; EP 10426 A HCAPLUS
  - (3) Eli Lilly And Co; EP 20836 A HCAPLUS
  - (4) Eli Lilly And Co; EP 29658 A HCAPLUS
  - (5) Eli Lilly And Co; US 4210647 A HCAPLUS
- ALL CITATIONS AVAILABLE IN THE RE FORMAT

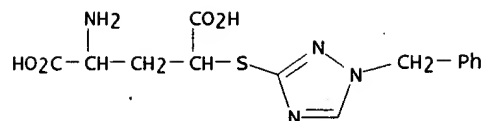
=&gt; d bib abs hitstr 134 2

L34 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1997:15490 HCAPLUS  
 DN 126:60367  
 TI Preparation of aryloxy- and arylthioglutamic acids as excitatory amino acid receptor antagonists  
 IN Heinz, Lawrence J.; Lunn, William H. W.; Schoepp, Darryle D.  
 PA Eli Lilly and Company, USA  
 SO U.S., 31 pp. Cont.-in-part of U.S. Ser. No. 161,830, abandoned.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 2

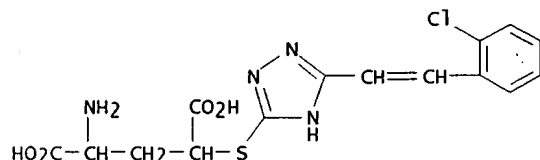
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5576323	A	19961119	US 1994-322632	19941013
	ZA 9409405	A	19960528	ZA 1994-9405	19941128
	NO 9404578	A	19950606	NO 1994-4578	19941129
	AU 9479151	A1	19950608	AU 1994-79151	19941130
	AU 676781	B2	19970320		
	BR 9404809	A	19950801	BR 1994-4809	19941201
	FI 9405704	A	19950604	FI 1994-5704	19941202
	EP 658539	A1	19950621	EP 1994-308949	19941202
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	HU 69181	A2	19950828	HU 1994-3469	19941202
	CN 1108240	A	19950913	CN 1994-119360	19941202
	JP 07267908	A2	19951017	JP 1994-299390	19941202
US 5843997	A	19981201	US 1996-626447	19960402	
PRAI	US 1993-161830		19931203		
	US 1994-322632		19941013		
OS	MARPAT 126:60367				
AB	Novel compds. R3pX3mX2sX1nCH(CO2R2)(CH2)rCH(NH2)CO2R1 [R1, R2 = H, protective group, R3, X2 = (un)substituted aryl or heterocyclyl group, X1 = NH2 or substituted amino, O, S, X3 = alkylene, alkenediyl, oxoalkylene, oxyalkylene, etc., m, n, s = 0, 1, p = 0-3, q = 0-6, r = 1, 2] or their pharmaceutically acceptable salts were prepd. as antagonists of excitatory amino acid receptors. Thus, Me 3-hydroxy-2-pyrrolidone-5-carboxylate was prepd. in 4 steps from cyclopentadiene and benzyl N-hydroxycarbamate and etherified with phenol and treated with LiOH in H2O-THF to afford 4-phenoxyglutamic acid. The latter at 10 .mu.M concn. gave 88.0% displacement of 3H-glutamate binding from rat brain cell membranes. Formulation contg. the title compds. are given.				
IT	170012-43-8P 170012-44-9P 185320-03-0P RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of aryloxy- and arylthioglutamic acids as excitatory amino acid receptor antagonists)				
RN	170012-43-8 HCAPLUS				
CN	Glutamic acid, 4-[[4-(phenylmethyl)-4H-1,2,4-triazol-3-yl]thio]- (9CI) (CA INDEX NAME)				



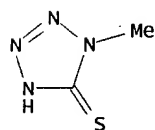
RN 170012-44-9 HCAPLUS  
 CN Glutamic acid, 4-[[1-(phenylmethyl)-1H-1,2,4-triazol-3-yl]thio]- (9CI)  
 (CA INDEX NAME)



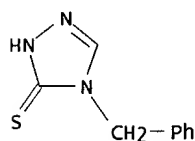
RN 185320-03-0 HCAPLUS  
 CN Glutamic acid, 4-[[5-[2-(2-chlorophenyl)ethenyl]-1H-1,2,4-triazol-3-yl]thio]- (9CI) (CA INDEX NAME)



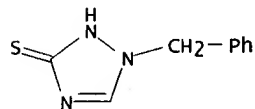
IT 13183-79-4, 1-Methyl-5-tetrazolethiol 23289-13-6  
 29983-25-3 185320-18-7  
 RL: RCT (Reactant)  
 (prepn. of aryloxy- and arylthioglutamic acids as excitatory amino acid receptor antagonists)  
 RN 13183-79-4 HCAPLUS  
 CN 5H-Tetrazole-5-thione, 1,2-dihydro-1-methyl- (9CI) (CA INDEX NAME)



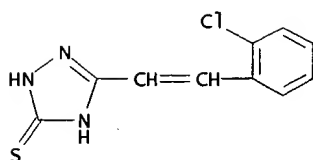
RN 23289-13-6 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 2,4-dihydro-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 29983-25-3 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 1,2-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 185320-18-7 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 5-[2-(2-chlorophenyl)ethenyl]-1,2-dihydro- (9CI) (CA INDEX NAME)

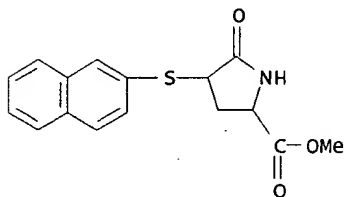


IT 170012-58-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of aryloxy- and arylthioglutamic acids as excitatory  
amino acid receptor antagonists)

RN 170012-58-5 HCAPLUS

CN Proline, 4-(2-naphthalenylthio)-5-oxo-, methyl ester (9CI) (CA INDEX  
NAME)

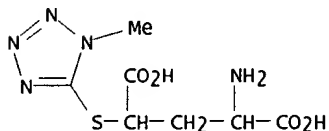


IT 170012-47-2P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological  
study); PREP (Preparation); USES (Uses)  
(prepn. of aryloxy- and arylthioglutamic acids as excitatory  
amino acid receptor antagonists)

RN 170012-47-2 HCAPLUS

CN Glutamic acid, 4-[(1-methyl-1H-tetrazol-5-yl)thio]- (9CI) (CA INDEX NAME)

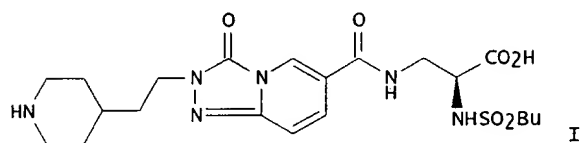




=&gt; d bib abs hitstr 134 3

L34 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1995:563209 HCAPLUS  
 DN 122:315095  
 TI Preparation of .omega.-[(heterocyclylcarbonyl)amino]-.alpha.-  
 amino acids and analogs as fibrinogen receptor  
 antagonists  
 IN Claremon, David Alan; Baldwin, John J.; Liverton, Nigel; Askew, Ben  
 PA Merck and Co., Inc., USA  
 SO PCT Int. Appl., 136 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9418981	A1	19940901	WO 1994-US1881	19940222
	W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US, UZ				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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	AU 9462465	A1	19940914	AU 1994-62465	19940222
	AU 680240	B2	19970724		
	EP 684823	A1	19951206	EP 1994-909745	19940222
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	HU 71796	A2	19960228	HU 1995-2028	19940222
	CN 1118139	A	19960306	CN 1994-191248	19940222
	JP 08507072	T2	19960730	JP 1994-519220	19940222
	US 5821241	A	19981013	US 1995-495560	19950801
	FI 9503916	A	19950821	FI 1995-3916	19950821
	NO 9503270	A	19951019	NO 1995-3270	19950821
PRAI	US 1993-20517		19930222		
	WO 1994-US1881		19940222		
OS	MARPAT 122:315095				
GI					

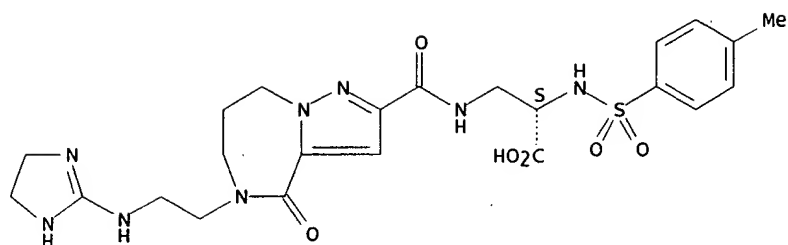


AB R(CH<sub>2</sub>)<sub>n</sub>Z<sub>1</sub>Z<sub>2</sub>CO<sub>2</sub>Z<sub>3</sub>Z<sub>4</sub>CR<sub>1</sub>R<sub>6</sub>R<sub>8</sub> [R = C(:NH)NH<sub>2</sub>, NHC(:NH)NH<sub>2</sub>, (alkyl)amino, heterocyclyl, etc.; R<sub>1</sub> = H, alkyl, (di)(alkyl)amino, NHSO<sub>2</sub>R<sub>7</sub>, etc.; R<sub>6</sub> = CO<sub>2</sub>H, CH<sub>2</sub>OH, P(O)(OH)<sub>2</sub>, etc.; R<sub>7</sub> = H, alk(en)yl, (hetero)aryl, etc.; R<sub>8</sub> = H, alkyl; Z<sub>1</sub> = bond, NR<sub>7</sub>CO; Z<sub>2</sub> = bicyclic heterocyclylene; Z<sub>3</sub> = bond, NR<sub>4</sub>; R<sub>4</sub> = H, (cyclo)alkyl, alkenyl; Z<sub>4</sub> = bond, CHR<sub>2</sub>(CH<sub>2</sub>)<sub>n</sub>; Z<sub>4</sub> = CO(CH<sub>2</sub>)<sub>n</sub> when Z<sub>3</sub> = NR<sub>4</sub>; R<sub>2</sub> = H, alkyl, (alkyl)aryl; n = 0-7] were prep'd. as fibrinogen receptor antagonists (no data). Thus, tert-Bu 2,3-dihydro-3-oxo-1,4-triazolo[4,3-a]pyridine-6-carboxylate (prepn. from tert-Bu 6-chloronicotinate given) was N-alkylated by 2-(N-benzyloxycarbonyl-4-piperidyl)ethyl iodide (prepn. given) and the sapond. product amidated by (S)-BuSO<sub>2</sub>NHCH(CH<sub>2</sub>NH<sub>2</sub>)CO<sub>2</sub>H (prepn. given) to give, after deprotection, title compd. I.

IT 163212-42-8P 163212-76-8P 163213-12-5P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of .omega.-[(heterocyclylcarbonyl)amino]-.alpha.-  
 amino acids and analogs as fibrinogen  
 receptor antagonists)

RN 163212-42-8 HCAPLUS  
 CN L-Alanine, 3-[[[5-[2-[(4,5-dihydro-1H-imidazol-2-yl)amino]ethyl]-5,6,7,8-tetrahydro-4-oxo-4H-pyrazolo[1,5-a][1,4]diazepin-2-yl]carbonyl]amino]-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

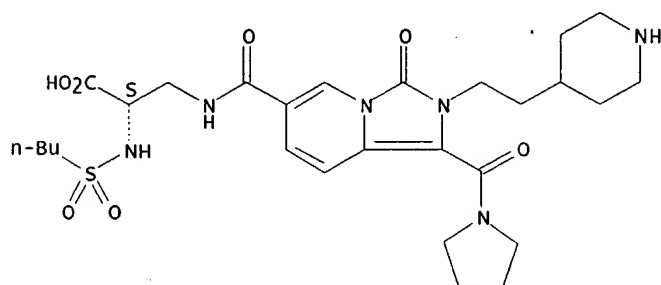
Absolute stereochemistry.



RN 163212-76-8 HCAPLUS

CN L-Alanine, N-(butylsulfonyl)-3-[[[2,3-dihydro-3-oxo-2-[2-(4-piperidiny)ethyl]-1-(1-pyrrolidinylcarbonyl)imidazo[1,5-a]pyridin-6-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

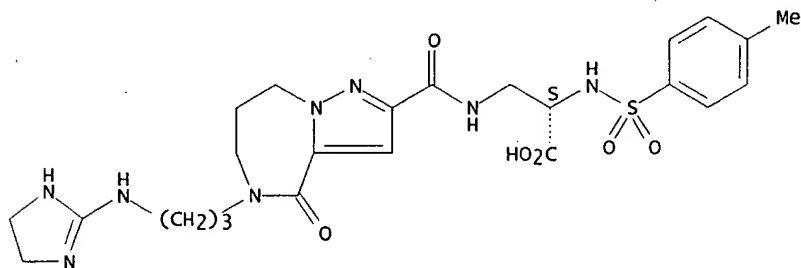
Absolute stereochemistry.



RN 163213-12-5 HCAPLUS

CN L-Alanine, 3-[[[5-[3-[(4,5-dihydro-1H-imidazol-2-yl)amino]propyl]-5,6,7,8-tetrahydro-4-oxo-4H-pyrazolo[1,5-a][1,4]diazepin-2-yl]carbonyl]amino]-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 40322-87-0, 2-Methylthio-2-imidazoline hydroiodide

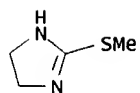
RL: RCT (Reactant)

(prepn. of .omega.-[(heterocyclylcarbonyl)amino]-.alpha.-amino acids and analogs as fibrinogen receptor antagonists)

RN 40322-87-0 HCAPLUS

CN 1H-Imidazole, 4,5-dihydro-2-(methylthio)-, hydriodide (9CI) (CA INDEX NAME)

CHOI 09/387,135



● x HI

=&gt; d bib abs hitstr l15 1

L15 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2001 ACS

AN 1999:335459 HCAPLUS

DN 131:125342

TI (R,S)-4-phosphonophenylglycine, a potent and selective group III metabotropic glutamate receptor agonist, is anticonvulsive and neuroprotective in vivo

AU Gasparini, F.; Bruno, V.; Battaglia, G.; Lukic, S.; Leonhardt, T.; Inderbitzin, W.; Laurie, D.; Sommer, B.; Varney, M. A.; Hess, S. D.; Johnson, E. C.; Kuhn, R.; Urwyler, S.; Sauer, D.; Portet, C.; Schmutz, M.; Nicoletti, F.; Flor, P. J.

CS Nervous System Research, Novartis Pharma AG, Basel, Switz.

SO J. Pharmacol. Exp. Ther. (1999), 289(3), 1678-1687

CODEN: JPETAB; ISSN: 0022-3565

PB American Society for Pharmacology and Experimental Therapeutics

DT Journal

LA English

AB Group III metabotropic glutamate receptors (mGluRs) are thought to modulate neurotoxicity of excitatory amino acids, via mechanisms of presynaptic inhibition, such as regulation of neurotransmitter release. Here, we describe (R,S)-4-phosphonophenylglycine (PPG) as a novel, potent, and selective agonist for group III mGluRs. In recombinant cell lines expressing the human receptors hmGluR4a, hmGluR6, hmGluR7b, or hmGluR8a, EC50 values for (R,S)-PPG of 5.2+-0.7 .mu.M, 4.7+-0.9 .mu.M, 185+-42 .mu.M, and 0.2+-0.1 .mu.M, resp., were measured. The compd. showed EC50 and IC50 values of .gtoreq.200 .mu.M at group I and II hmGluRs and was inactive at cloned human N-methyl-D-aspartate, .alpha.-amino-3-hydroxy-5-methyl-isoxazole-4-propionate, and kainate receptors (>300 .mu.M). On the other hand, it showed micromolar affinity for a Ca2+/Cl--dependent L-glutamate binding site in rat brain, similar to other phosphono-substituted amino acids like L-2-amino-4-phosphonobutyrate. In cultured cortical neurons, (R,S)-PPG provided protection against a toxic pulse of N-methyl-D-aspartate (EC50 = 12 .mu.M), which was reversed by the group III mGluR antagonist (R,S)-.alpha.-methylserine-O-phosphate but not by the group II antagonist (2S)-.alpha.-ethylglutamate. Moreover, (R,S)-PPG protected against N-methyl-D-aspartate- and quinolinic acid-induced striatal lesions in rats and was anticonvulsive in the maximal electroshock model in mice. In contrast to the group III mGluR agonists L-2-amino-4-phosphonobutyrate and L-serine-O-phosphate, (R,S)-PPG showed no proconvulsive effects (2200 nmol i.c.v.). These data provide novel in vivo evidence for group III mGluRs as attractive targets for neuroprotective and anticonvulsive therapy. Also, (R,S)-PPG represents an attractive tool to analyze the roles of group III mGluRs in nervous system physiol. and pathol.

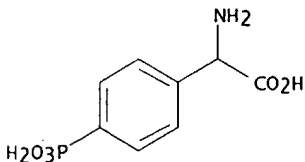
IT 120667-15-4P

RL: BAC (Biological activity or effector, except adverse); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

((R,S)-4-phosphonophenylglycine anticonvulsive and neuroprotective activity, and relation to group III metabotropic glutamate receptors)

RN 120667-15-4 HCAPLUS

CN Benzeneacetic acid, .alpha.-amino-4-phosphono- (9CI) (CA INDEX NAME)



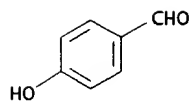
IT 123-08-0, 4-Hydroxybenzaldehyde

RL: RCT (Reactant)

(reaction; (R,S)-4-phosphonophenylglycine anticonvulsive and neuroprotective activity, and relation to group III metabotropic glutamate receptors)

RN 123-08-0 HCAPLUS

CN Benzaldehyde, 4-hydroxy- (9CI) (CA INDEX NAME)



RE.CNT 41

RE

- (1) Abdul-Ghani, A; Brain Res 1997, V755, P202 HCAPLUS
- (2) Bedingfield, J; Eur J Pharmacol 1996, V309, P71 HCAPLUS
- (3) Bigge, C; J Med Chem 1989, V32, P1580 HCAPLUS
- (4) Bruno, V; Eur J Pharmacol 1996, V310, P61 HCAPLUS
- (5) Colwell, C; Brain Res 1996, V726, P223 HCAPLUS

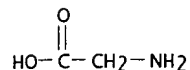
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; d bib abs hitstr 115 2

L15 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1998:700733 HCAPLUS  
 DN 130:61231  
 TI The human N-methyl-D-aspartate receptor 2C subunit: genomic analysis, distribution in human brain, and functional expression  
 AU Daggett, L. P.; Johnson, E. C.; Varney, M. A.; Lin, F.-F.; Hess, S. D.; Deal, C. R.; Jachec, C.; Lu, C.-C.; Kerner, J. A.; Landwehrmeyer, G. B.; Standaert, D. G.; Young, A. B.; Harpold, M. M.; Velicelebi, G.  
 CS SIBIA Neurosciences, Inc., La Jolla, CA, 92037, USA  
 SO J. Neurochem. (1998), 71(5), 1953-1968  
 CODEN: JONRA9; ISSN: 0022-3042  
 PB Lippincott-Raven Publishers  
 DT Journal  
 LA English  
 AB The cDNAs encoding four isoforms of the human NMDA receptor (NMDAR) NMDAR2C (hNR2C-1, -2, -3, and -4) have been isolated and characterized. The overall identity of the deduced amino acid sequences of human and rat NR2C-1 is 89.0%. The sequences of the rat and human C-termini (Gly925-Val1,236) are encoded by different exons and are only 71.5% homologous. In situ hybridization in human brain revealed the expression of the NR2C mRNA in the pontine reticular formation and lack of expression in substantia nigra pars compacta in contrast to the distribution pattern obsd. previously in rodent brain. The pharmacol. properties of hNR1A/2C were detd. by measuring agonist-induced inward currents in Xenopus oocytes and compared with those of other human NMDAR subtypes. Glycine, glutamate, and NMDA each discriminated between hNR1A/2C-1 and at least one of hNR1A/2A, hNR1A/2B, or hNR1A/2D subtypes. Among the antagonists tested, CGS 19755 did not significantly discriminate between any of the four subtypes, whereas 5,7-dichlorokynurenic acid distinguished between hNR1A/2C and hNR1A/2D. Immunoblot anal. of membranes isolated from HEK293 cells transiently transfected with cDNAs encoding hNR1A and each of the four NR2C isoforms indicated the formation of heteromeric complexes between hNR1A and all four hNR2C isoforms. HEK293 cells expressing hNR1A/2C-3 or hNR1A/2C-4 did not display agonist responses. In contrast, the authors obsd. an agonist-induced elevation of intracellular free calcium and whole-cell currents in cells expressing hNR1A/2C-1 or hNR1A/2C-2. There were no detectable differences in the macroscopic biophys. properties of hNR1A/2C-1 or hNR1A/2C-2.  
 IT 7440-70-2, Calcium, biological studies  
 RL: BPR (Biological process); BIOL (Biological study); PROC (Process) (NMDA receptor 2C subunit sequencing and genomic anal., distribution in human brain, and functional expression)  
 RN 7440-70-2 HCAPLUS  
 CN Calcium (8CI, 9CI) (CA INDEX NAME)

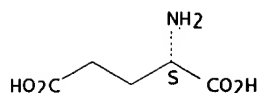
Ca

IT 56-40-6, Glycine, biological studies 56-86-0, L-Glutamic acid, biological studies 6384-92-5, NMDA 131123-76-7, 5,7-Dichlorokynurenic acid  
 RL: BPR (Biological process); BUU (Biological use, unclassified); BIOL (Biological study); PROC (Process); USES (Uses) (NMDA receptor 2C subunit sequencing and genomic anal., distribution in human brain, and functional expression)  
 RN 56-40-6 HCAPLUS  
 CN Glycine (8CI, 9CI) (CA INDEX NAME)



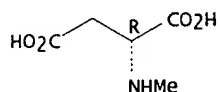
RN 56-86-0 HCAPLUS  
 CN L-Glutamic acid (9CI) (CA INDEX NAME)

Absolute stereochemistry.

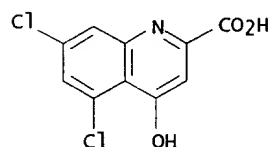


RN 6384-92-5 HCAPLUS  
CN D-Aspartic acid, N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 131123-76-7 HCAPLUS  
CN 2-Quinolinecarboxylic acid, 5,7-dichloro-4-hydroxy- (9CI) (CA INDEX NAME)



IT 217638-85-2  
RL: PRP (Properties)  
(amino acid sequence; NMDA receptor 2C subunit sequencing and genomic anal., distribution in human brain, and functional expression)  
RN 217638-85-2 HCAPLUS  
CN NMDA receptor (human clone hNMDAR2C-1 NR2C-1-subunit precursor) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

IT 197348-40-6, GenBank U77782  
RL: PRP (Properties)  
(nucleotide sequence; NMDA receptor 2C subunit sequencing and genomic anal., distribution in human brain, and functional expression)  
RN 197348-40-6 HCAPLUS  
CN DNA (human clone hNMDAR2C-1 NMDA receptor NR2C-1-subunit cDNA plus flanks) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RE.CNT 43

RE

- (1) Adams, S; Biochim Biophys Acta 1995, V1260, P105 HCAPLUS
- (2) Bliss, T; Nature 1993, V361, P31 HCAPLUS
- (3) Buller, A; Mol Pharmacol 1995, V48, P717 HCAPLUS
- (5) Counihan, T; J Comp Neurol 1998, V390, P91 HCAPLUS
- (6) Daggett, L; Neuropharmacology 1995, V34, P871 HCAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; d bib abs hitstr 115 3

L15 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1995:452110 HCAPLUS  
 DN 122:257079  
 TI Human metabotropic glutamate receptor subtypes and cDNAs encoding them and their use in the study of receptor agonists and antagonists  
 IN Daggett, Lorrie; Ellis, Steven B.; Liaw, Chen; Pontsler, Aaron; Johnson, Edwin C.; Hess, Stephen D.  
 PA Salk Institute Biotechnology/Industrial Associates, Inc., USA  
 SO PCT Int. Appl., 126 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9429449	A1	19941222	WO 1994-US6273	19940603
	W: AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KG, KP, KR, KZ, LK, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 5521297	A	19960528	US 1993-72574	19930604
	CA 2161811	AA	19941222	CA 1994-2161811	19940603
	AU 9470989	A1	19950103	AU 1994-70989	19940603
	AU 685471	B2	19980122		
	GB 2286398	A1	19950816	GB 1995-3691	19940603
	GB 2286398	B2	19971015		
	EP 701611	A1	19960320	EP 1994-920075	19940603
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 08511168	T2	19961126	JP 1994-501975	19940603
	US 5807689	A	19980915	US 1995-486270	19950606
PRAI	US 1993-72574		19930604		
	WO 1994-US6273		19940603		
	US 1995-367264		19950109		
AB	CDNAs encoding human metabotropic glutamate receptor subtypes mGluR1, mGluR3 and mGluR5 and the proteins encoded by them are characterized for use in the study of receptor biol. In addn. to being useful for the manuf. of metabotropic glutamate receptor subtypes, the nucleic acids may also be used as probes to identify and isolate related human receptor subunits. These receptors can also be used to identify agonists and antagonists of the receptor subtypes. The cDNAs were cloned from human brain tissue cDNA libraries by screening with corresponding rat cDNAs; at least one of the cDNAs was obtained by assembling overlapping partial clones. The mGluR5 cDNA sequence indicated the presence of alternative splicing variants. Expression of the cDNAs was achieved in animal cell lines with transgenic cells showing receptor activity.				
IT	162393-88-6 162393-89-7 162535-82-2 162535-84-4 162535-85-5 162535-86-6 162535-87-7 162535-88-8				
	RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence) (amino acid sequence; human metabotropic glutamate receptor subtypes and cDNAs encoding them and their use in study of receptor agonists and antagonists)				
RN	162393-88-6 HCAPLUS				
CN	Receptor, glutamatergic (human clone METAB58 gene GluR1) (9CI) (CA INDEX NAME)				

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 162393-89-7 HCAPLUS

CN Receptor, glutamatergic (human clone METAB40 gene GluR2 fragment) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 162535-82-2 HCAPLUS

CN Receptor, glutamatergic (human clone METAB45 gene GluR3) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 162535-84-4 HCAPLUS

CN Receptor, glutamatergic (human clone METAB1 gene GluR5 isoform R5a1) (9CI) (CA INDEX NAME)



\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 162535-85-5 HCAPLUS

CN DNA (human clone METAB1 metabotropic glutamatergic receptor 5 isoform 5b cDNA plus flanks) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 162535-86-6 HCAPLUS

CN Receptor, glutamatergic (human clone METAB1 gene GluR5 isoform R5b) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 162535-87-7 HCAPLUS

CN DNA (human clone METAB1 metabotropic glutamatergic receptor 5 isoform 5c cDNA plus flanks) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 162535-88-8 HCAPLUS

CN Receptor, glutamatergic (human clone METAB1 gene GluR5 isoform R5c) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

IT 162078-65-1 162393-87-5 162393-90-0

162535-83-3

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)  
(nucleotide sequence; human metabotropic glutamate receptor subtypes and cDNAs encoding them and their use in study of receptor agonists and antagonists)

RN 162078-65-1 HCAPLUS

CN DNA (human clone METAB40 metabotropic glutamatergic receptor 2-specifying) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 162393-87-5 HCAPLUS

CN DNA (human clone METAB58 metabotropic glutamatergic receptor 1B cDNA plus flanks) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 162393-90-0 HCAPLUS

CN DNA (human clone METAB48 metabotropic glutamatergic receptor 3 cDNA plus flanks) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 162535-83-3 HCAPLUS

CN DNA (human clone METAB1 metabotropic glutamatergic receptor 5 isoform 5a1 cDNA plus flanks) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

IT 162535-89-9

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(nucleotide sequence; human metabotropic glutamate receptor subtypes and cDNAs encoding them and their use in study of receptor agonists and antagonists)

RN 162535-89-9 HCAPLUS

CN DNA (human clone METAB40 metabotropic glutamatergic receptor 2 gene 3'-flank) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

=&gt; d bib abs hitstr 115 4

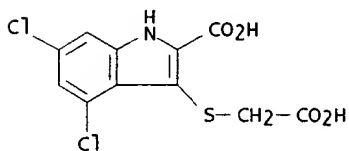
L15 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1993:531539 HCAPLUS  
 DN 119:131539  
 TI Potentiation of NMDA antagonists with probenecid  
 IN McDonald, Ian A.; Baron, Bruce M.  
 PA Merrell Dow Pharmaceuticals, Inc., USA  
 SO PCT Int. Appl., 26 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9312780	A1	19930708	WO 1992-US10354	19921201
	W: AU, CA, JP, KR, NZ				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 5318985	A	19940607	US 1991-811204	19911220
	AU 9331509	A1	19930728	AU 1993-31509	19921201
	AU 667333	B2	19960321		
	EP 617616	A1	19941005	EP 1992-925469	19921201
	EP 617616	B1	19991027		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 07504890	T2	19950601	JP 1992-511664	19921201
	AT 185969	E	19991115	AT 1992-925469	19921201
	US 5489579	A	19960206	US 1994-191996	19940204
PRAI	US 1991-811204		19911220		
	WO 1992-US10354		19921201		
OS	MARPAT 119:131539				
AB	Probenecid potentiates the therapeutic activity of known antagonists of NMDA receptor-excitatory amino acids. The antagonists comprise 4 classes of compds. (Markush structures given), such as carboxyindoles, phosphonates and carboxypiperidines. The compns. comprising probenecid and the antagonists are useful for the treatment of epilepsy, neurodegenerative diseases, anxiety, etc. Probenecid potentiated the ability of (R)-4-oxo-5-phosphononorvaline to inhibit quinolinic acid-induced clonic seizures in mice.				
IT	149890-43-7 149890-44-8				
	RL: BIOL (Biological study)				
	(antiepileptic)				
RN	149890-43-7 HCAPLUS				
CN	1H-Indole-2-carboxylic acid, 3-[(carboxymethyl)thio]-4,6-dichloro-, mixt. with 4-[(diisopropylamino)sulfonyl]benzoic acid (9CI) (CA INDEX NAME)				

CM 1

CRN 137836-29-4

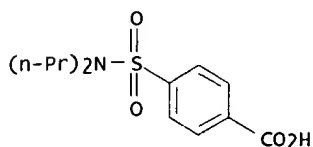
CMF C11 H7 C12 N O4 S



CM 2

CRN 57-66-9

CMF C13 H19 N O4 S

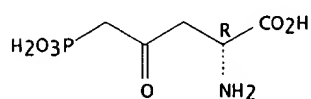


RN 149890-44-8 HCAPLUS  
 CN D-Norvaline, 4-oxo-5-phosphono-, mixt. with 4-  
 [(dipropylamino)sulfonyl]benzoic acid (9CI) (CA INDEX NAME)

CM 1

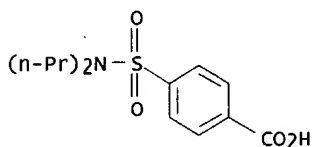
CRN 129938-34-7  
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 CDES 5:D

Absolute stereochemistry.

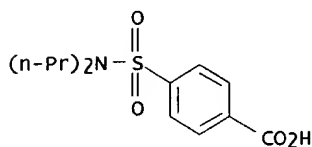


CM 2

CRN 57-66-9  
 CMF C13 H19 N O4 S



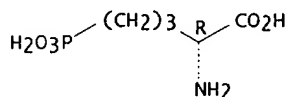
IT 57-66-9D, Probenecid, mixt. with antagonists of NMDA  
 receptor-excitatory amino acids  
 RL: BIOL (Biological study)  
 (epilepsy and neurodegenerative diseases treatment by)  
 RN 57-66-9 HCAPLUS  
 CN Benzoic acid, 4-[(dipropylamino)sulfonyl]- (9CI) (CA INDEX NAME)



=&gt; d bib abs hitstr 115 5

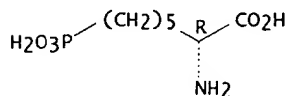
L15 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1992:227662 HCAPLUS  
 DN 116:227662  
 TI Modeling of competitive phosphono amino acid NMDA  
 receptor antagonists  
 AU Whitten, Jeffrey P.; Harrison, Boyd L.; Weintraub, Herschel J. R.;  
 McDonald, Ian A.  
 CS Marion Merrell Dow Res. Inst., Cincinnati, OH, 45215, USA  
 SO J. Med. Chem. (1992), 35(9), 1509-14  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DT Journal  
 LA English  
 AB A pharmacophore for the phosphono amino acid  
 antagonists of the NMDA receptor was developed using  
 computer-based mol. modeling techniques. An important feature of this  
 model is that a single binding site is proposed for the phosphonic acid  
 moiety. All competitive antagonists examd. incorporating amino acid and  
 phosphonate groups in their structure fit the pharmacophore in  
 energetically accessible conformations.  
 IT 79055-68-8 81338-23-0 110347-85-8  
 113190-89-9 113190-92-4 113229-88-2  
 121524-85-4 121524-86-5 121524-87-6  
 121570-54-5 121570-55-6 121570-57-8  
 127910-31-0 131177-53-2 141039-92-1  
 RL: PROC (Process)  
 (binding of, to NMDA receptors, pharmacophore model for)  
 RN 79055-68-8 HCAPLUS  
 CN D-Norvaline, 5-phosphono- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



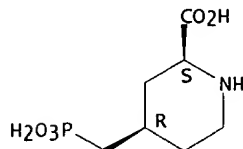
RN 81338-23-0 HCAPLUS  
 CN Heptanoic acid, 2-amino-7-phosphono-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



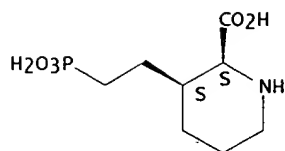
RN 110347-85-8 HCAPLUS  
 CN 2-Piperidinecarboxylic acid, 4-(phosphonomethyl)-, (2R,4S)-rel- (9CI) (CA  
 INDEX NAME)

Relative stereochemistry.



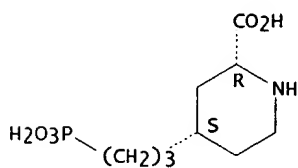
RN 113190-89-9 HCAPLUS  
 CN 2-Piperidinecarboxylic acid, 3-(2-phosphonoethyl)-, cis- (9CI) (CA INDEX  
 NAME)

Relative stereochemistry.



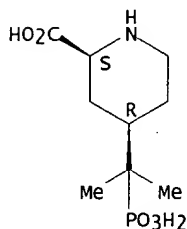
RN 113190-92-4 HCAPLUS  
CN 2-Piperidinecarboxylic acid, 4-(3-phosphonopropyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

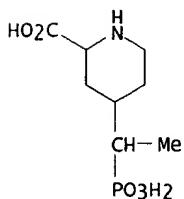


RN 113229-88-2 HCAPLUS  
CN 2-Piperidinecarboxylic acid, 4-(1-methyl-1-phosphonoethyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

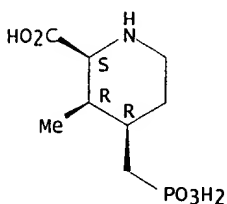


RN 121524-85-4 HCAPLUS  
CN 2-Piperidinecarboxylic acid, 4-(1-phosphonoethyl)- (9CI) (CA INDEX NAME)



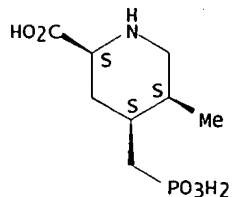
RN 121524-86-5 HCAPLUS  
CN 2-Piperidinecarboxylic acid, 3-methyl-4-(phosphonomethyl)-, (2.alpha.,3.alpha.,4.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



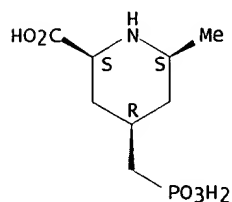
RN 121524-87-6 HCAPLUS  
 CN 2-Piperidinecarboxylic acid, 5-methyl-4-(phosphonomethyl)-,  
 (2.alpha.,4.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



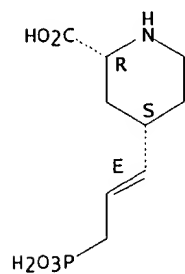
RN 121570-54-5 HCAPLUS  
 CN 2-Piperidinecarboxylic acid, 6-methyl-4-(phosphonomethyl)-,  
 (2.alpha.,4.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



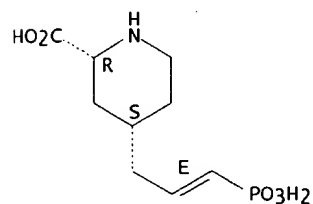
RN 121570-55-6 HCAPLUS  
 CN 2-Piperidinecarboxylic acid, 4-(3-phosphono-1-propenyl)-,  
 [2.alpha.,4.alpha.(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.



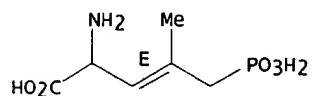
RN 121570-57-8 HCAPLUS  
 CN 2-Piperidinecarboxylic acid, 4-(3-phosphono-2-propenyl)-,  
 [2.alpha.,4.alpha.(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.



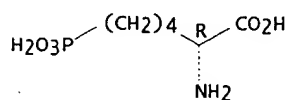
RN 127910-31-0 HCAPLUS  
 CN 3-Pentenoic acid, 2-amino-4-methyl-5-phosphono-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



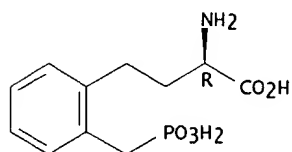
RN 131177-53-2 HCAPLUS  
 CN D-Norleucine, 6-phosphono- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 141039-92-1 HCAPLUS  
 CN Benzenebutanoic acid, .alpha.-amino-2-(phosphonomethyl)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=&gt; d bib abs hitstr 115 6

L15 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2001 ACS

AN 1991:17877 HCAPLUS

DN 114:17877

TI Activity of 5,7-dichlorokynurenic acid, a potent antagonist at the N-methyl-D-aspartate receptor-associated glycine binding site

AU Baron, Bruce M.; Harrison, Boyd L.; Miller, Francis P.; McDonald, Ian A.; Salituro, Francesco G.; Schmidt, Christopher J.; Sorensen, Stephen M.; White, H. Steven; Palfreyman, Michael G.

CS Merrell Dow Res. Inst., Cincinnati, OH, 45215, USA

SO Mol. Pharmacol. (1990), 38(4), 554-61

CODEN: MOPMA3; ISSN: 0026-895X

DT Journal

LA English

AB 5,7-Dichlorokynurenic acid (5,7-DCKA), one of the most potent excitatory amino acid receptor antagonists yet described, binds to a strychnine-insensitive glycine binding site located on the N-methyl-D-aspartate (NMDA) receptor complex ( $K_i = 79$  nM vs.  $[^3H]$ glycine). 5,7-DCKA ( $10 \mu\text{M}$ ) antagonized the ability of NMDA to stimulate the binding of the radiolabeled ion channel blocker N- $[^3H]$ -[1-(2-thienyl)cyclohexyl]-piperidine ( $[^3H]$ TCP). Glycine overcame this effect and in the presence of 5,7-DCKA enhanced  $[^3H]$ TCP binding to antagonist-free levels. 5,7-DCKA completely and noncompetitively antagonized several NMDA receptor-mediated biochem. and electrophysiol. responses. Thus, micromolar concns., 5,7-DCKA inhibited: NMDA-stimulated elevation of cytosolic Ca in cultured hippocampal neurons, cGMP accumulation in cerebellar slices, and norepinephrine release from hippocampal slices. The glycine antagonist could also block the action of synaptically released agonist, as shown by its ability to inhibit the increase in the magnitude of the population spike that follows tetanic stimulation of the hippocampus in vitro (long term potentiation). Inclusion of glycine or D-serine prevented all these effects of the antagonist. 5,7-DCKA was a potent anticonvulsant when administered intracerebroventricularly to mice. As in the in vitro expts. the dose-response curve for the antagonist was shifted rightward in a parallel fashion when D-serine was coinjected. This spectrum of activity displayed by a compd. acting at the glycine binding site suggests that the therapeutic utility of glycine antagonists will be similar to those proposed for other types of glutamate receptor antagonists.

IT 7665-99-8, CGMP

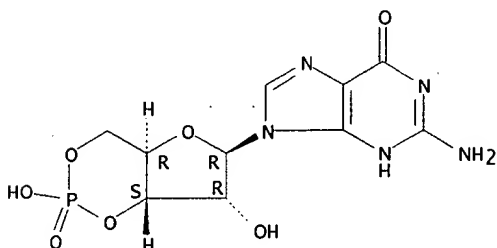
RL: BIOL (Biological study)

(accumulation of, by cerebellum, dichlorokynurenate effect on)

RN 7665-99-8 HCAPLUS

CN Guanosine, cyclic 3',5'-(hydrogen phosphate) (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 131123-76-7

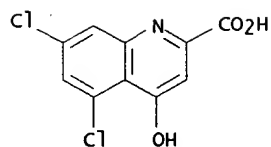
RL: BIOL (Biological study)

(methylaspartate receptor binding of glycine antagonism by)

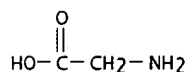
RN 131123-76-7 HCAPLUS

CN 2-Quinolincarboxylic acid, 5,7-dichloro-4-hydroxy- (9CI) (CA INDEX NAME)



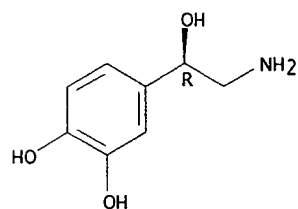


IT 56-40-6, Glycine, biological studies  
 RL: BIOL (Biological study)  
 (methylaspartate receptor binding of, dichlorokynurenine antagonism of)  
 RN 56-40-6 HCAPLUS  
 CN Glycine (8CI, 9CI) (CA INDEX NAME)



IT 51-41-2, Norepinephrine  
 RL: BIOL (Biological study)  
 (release of, by hippocampus, dichlorokynurenate and glycine effect on)  
 RN 51-41-2 HCAPLUS  
 CN 1,2-Benzenediol, 4-[(1R)-2-amino-1-hydroxyethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 7440-70-2, Calcium, biological studies  
 RL: BIOL (Biological study)  
 (transport of, by hippocampus, dichlorokynurenate effect on)  
 RN 7440-70-2 HCAPLUS  
 CN Calcium (8CI, 9CI) (CA INDEX NAME)

Ca

=&gt; d bib abs hitstr

L16 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2001 ACS  
 AN 2001:167983 HCAPLUS  
 TI Heterocyclic compounds and methods of use thereof  
 IN Cosford, Nicholas D. P.; McDonald, Ian A.; Bleicher,  
 Leo Solomon; Cube, Rowena V.; Schweiger, Edwin J.; Vernier, Jean-Michel;  
 Hess, Stephen D.; Varney, Mark A.; Munoz, Benito  
 PA Merck & Co., Inc., USA  
 SO PCT Int. Appl., 132 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001016121	A1	20010308	WO 2000-US23923	20000831
	W:				AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
	RW:				GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI	US 1999-387073		19990831		
	US 1999-387135		19990831		
AB	<p>In accordance with the present invention, there are provided novel class of heterocyclic compounds and methods of use thereof. Compounds of the invention contain a substituted, unsaturated five, six or seven membered heterocyclic ring that includes at least one nitrogen atom and at least one carbon atom. At a ring position adjacent to a ring nitrogen atom, the heterocyclic ring has at least one substituent which includes a moiety, linked to the heterocyclic ring via an alkylene moiety, an alkynylene moiety or an azo group. Invention compounds are capable of a wide variety of uses including modulating physiological processes by functioning as agonists and antagonists of receptors in the nervous system, as insecticides, and as fungicides. The invention further provides methods of modulating the activity of excitatory amino acid receptors using a specifically defined class of heterocyclic compounds including the novel compounds referred to above. In one embodiment, there are provided methods of modulating metabotropic glutamate receptors. The present invention also discloses methods of treating disease using heterocyclic compounds. The invention further discloses methods of preventing disease conditions related to diseases of the pulmonary system, diseases of the nervous system, diseases of the cardiovascular system, diseases of the gastrointestinal system, diseases of the endocrine system, diseases of the exocrine system, diseases of the skin, cancer and diseases of the ophthalmic system. The invention also discloses pharmaceutically acceptable salt forms of the above-described heterocyclic compounds.</p>				

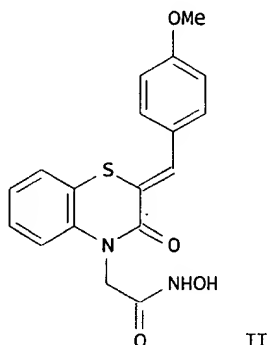
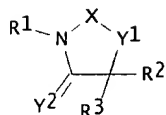
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L16 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2001 ACS  
 IC ICM C07D277-22  
 ICS C07D277-24; C07D277-40; C07D213-16; C07D213-30; C07D239-26;  
 C07D263-32; C07D271-06; C07D241-12; C07D249-08; C07D285-00;  
 C07D333-08; C07D417-06; C07D409-06; C07D407-06  
 CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))

=&gt; d bib abs hitstr 154 1

L54 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2001 ACS  
 AN 2000:756696 HCAPLUS  
 DN 133:321892  
 TI Preparation of hydroxamic acid derivatives as matrix metallo-proteinase inhibitors  
 IN Scarlato, Gerard Robert; Hadida, Ruah Sara Sabina; Nishimura, Tamiki; Nakatsuka, Masashi; Samizo, Fumio; Kamikawa, Yumiko; Houtigai, Hitoshi  
 PA Sumitomo Pharmaceuticals Co., Ltd., Japan; Hadida Ruah, Sara Sabina  
 SO PCT Int. Appl., 218 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

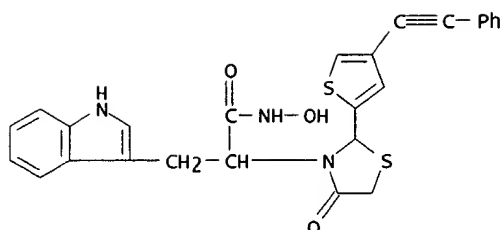
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000063197	A1	20001026	WO 2000-US10383	20000419
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
PRAI	US 1999-129933		19990419		
OS	MARPAT 133:321892				
GI					



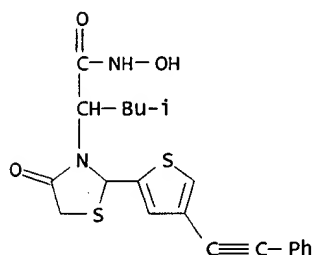
AB The title compds. [I; X = (un)substituted alkylene, ortho-heteroarylene; Y1 = O, S, SO2; Y2 = O, S; one of R1 and R3 = (CHR4)nCR5R6CONHOH; the other R1 and R3 = H, (un)substituted alkyl, cycloalkyl; R2 = H, (un)substituted alkyl, alkenyl, etc.; R4-R6 = H, (un)substituted alkyl, alkenyl, etc.; or R5 may be joined with R4 or R6 to form, with the carbon atom which they attach (un)substituted cycloalkane or heterocycloalkane; n = 0-4], useful as matrix metallo-proteinase (e.g., MMP-2, MMP-3, MMP-9, and MMP-13) inhibitors, were prepd. E.g., a multi-step synthesis of 1,4-benzothiazin-3(4H)-one II which showed IC50 of 1.0 .mu.M against MMP-2, and 20% inhibition of TNF-.alpha. prodn. at 5 .mu.M, was given.

IT 302827-22-1P 302827-33-4P 302827-58-3P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of hydroxamic acid derivs. as matrix metallo-proteinase inhibitors)

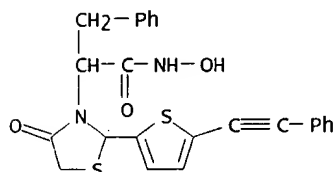
RN 302827-22-1 HCAPLUS  
 CN 1H-Indole-3-propanamide, N-hydroxy-.alpha.-[4-oxo-2-[4-(phenylethynyl)-2-thienyl]-3-thiazolidinyl]- (9CI) (CA INDEX NAME)



RN 302827-33-4 HCAPLUS  
 CN 3-Thiazolidineacetamide, N-hydroxy-.alpha.-(2-methylpropyl)-4-oxo-2-[4-(phenylethynyl)-2-thienyl]- (9CI) (CA INDEX NAME)



RN 302827-58-3 HCAPLUS  
 CN 3-Thiazolidineacetamide, N-hydroxy-4-oxo-2-[5-(phenylethynyl)-2-thienyl]-.alpha.-(phenylmethyl)- (9CI) (CA INDEX NAME)



RE.CNT 5  
 RE  
 (1) Ciba Geigy Ag; EP 0606046 A 1994 HCAPLUS  
 (2) Du Pont Merck Pharma; WO 9633176 A 1996 HCAPLUS  
 (3) Hoechst Ag; DE 19542189 A 1997 HCAPLUS  
 (4) Sunkyoung Ind Ltd; WO 9620936 A 1996 HCAPLUS  
 (5) Yoshitomi Pharmaceutical; FR 2434150 A 1980 HCAPLUS

=> d ind

LS6 HAS NO ANSWERS

'IND' IS NOT A VALID STRUCTURE FORMAT KEYWORD

Structure Formats

SIA ----- Structure Image, Attributes, and map table if it contains data. (Default)

SIM ----- Structure Image.

SAT ----- Structure Attributes and map table if it contains data.

SCT ----- Structure Connection Table and map table if it contains data.

SDA ----- All Structure Data (image, attributes, connection table and map table if it contains data).

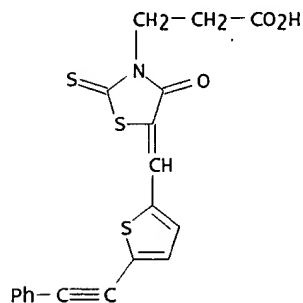
NOS ----- NO Structure data.

ENTER STRUCTURE FORMAT (SIA), SCT, SDA, SIM, SAT, NOS:end

=&gt; d bib abs hitstr 154 2

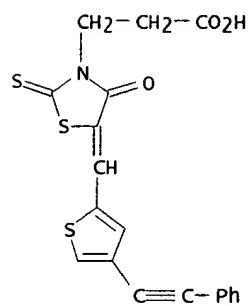
L54 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2001 ACS  
 AN 2000:144739 HCAPLUS  
 DN 132:189652  
 TI Rhodanine derivatives, preparation thereof, compositions, and methods for treating or preventing Flaviviridae family viral infections and associated diseases  
 IN Bailey, Thomas R.; Young, Dorothy C.  
 PA Viropharma Incorporated, USA  
 SO PCT Int. Appl., 91 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000010573	A1	20000302	WO 1999-US18785	19990819
	W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	AU 9955702	A1	20000314	AU 1999-55702	19990819
PRAI	US 1998-97476		19980821		
	US 1998-113212		19981222		
	US 1999-119328		19990209		
	US 1999-135585		19990524		
	US 1999-135586		19990524		
	WO 1999-US18785		19990819		
OS	MARPAT 132:189652				
AB	Compds., compns. and methods are provided for the treatment and prophylaxis of infections and assocd. diseases caused by viruses of the Flaviviridae family by administering certain rhodanine derivs., and analogs thereof, tri- and tetracyclic rhodanine alkanolic acids and rhodanine benzoic acids being particularly effective.				
IT	259811-82-0 259811-84-2 259812-05-0 RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (rhodanine derivs., prepn., compns., and methods for treating or preventing Flaviviridae family viral infections and assocd. diseases)				
RN	259811-82-0 HCAPLUS				
CN	3-Thiazolidinepropanoic acid, 4-oxo-5-[[5-(phenylethynyl)-2-thienyl]methylene]-2-thioxo- (9CI) (CA INDEX NAME)				

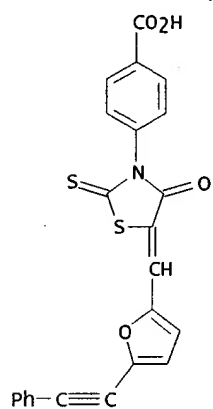


RN 259811-84-2 HCAPLUS  
 CN 3-Thiazolidinepropanoic acid, 4-oxo-5-[[4-(phenylethynyl)-2-thienyl]methylene]-2-thioxo- (9CI) (CA INDEX NAME)

CHOI 09/387,135



RN 259812-05-0 HCAPLUS  
CN Benzoic acid, 4-[4-oxo-5-[[5-(phenylethynyl)-2-furanyl]methylene]-2-thioxo-3-thiazolidinyl]- (9CI) (CA INDEX NAME)

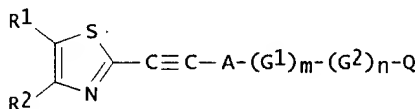


RE.CNT 6  
RE  
(1) Hughes; US 3888984 A 1975 HCAPLUS  
(2) Kawamatsu; US 4387101 A 1983 HCAPLUS  
(3) Ramasamy; US 5834466 A 1998 HCAPLUS  
(4) Schnur; US 4367234 A 1983 HCAPLUS  
(6) Suzuki; US 5693337 A 1997 HCAPLUS  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

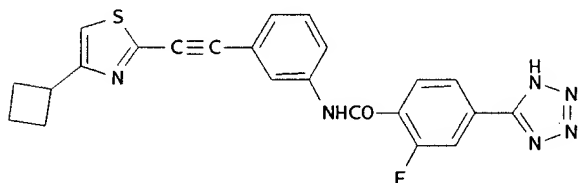
=&gt; d bib abs hitstr 154 3

L54 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1998:493329 HCAPLUS  
 DN 129:189329  
 TI Preparation of 2-ethynylthiazole derivatives as leukotriene antagonists  
 IN Nakayama, Atsushi; Takeda, Satoshi; Machinaga, Nobuo; Ogasawara, Tomomi;  
 Naito, Hiroshi; Hasegawa, Masashi; Haruda, Makoto  
 PA Daiichi Seiyaku Co., Ltd., Japan  
 SO Jpn. Kokai Tokkyo Koho, 121 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10195063	A2	19980728	JP 1997-286340	19971020
PRAI	JP 1996-278347		19961021		
OS	MARPAT 129:189329				
GI					



I



II

AB The title compds. [I; R1, R2 = H, halo, (un)substituted alkyl or cycloalkyl; or R1 and R2 together form a ring; A = (un)substituted Ph, pyridyl, furyl, thienyl, benzofuranyl, benzo[b]thienyl, benzoxazolyl, benzothiazolyl, pyrido[1,2-a]pyrimidinyl, quinazolyl, benzotriazinyl, or 2H-chromenyl; G1 = O, CO, C.tplbond.C, (un)substituted NR3CO, NR4, NR5SO2, SO2NR6, CONR7, C(:CHR8), CR9:CR10; R3 - R7 = H, OH, (un)substituted alkyl; R8 = cyano, CO2H, (un)substituted alkoxy carbonyl; R9, R10 = H, halo, (un)substituted alkyl, cycloalkyl, or aryl; or R9 and R10 together form a ring; G2 = (un)substituted Ph, pyridyl, thiazolyl, isoxazolyl, thienyl, or pyrimidinyl, etc.; m, n = 0, 1; Q = CO2H, (un)substituted alkoxy carbonyl, 5-tetrazolylaminocarbonyl, (un)substituted 5-tetrazolyl, 1,2,3-triazolyl, 2,4-dioxothiazolidin-5-ylidene, or 4-oxo-2-thioxothiazolidin-5-ylidene, etc.; excluding the case where m = n = 0 and Q = CO2H or alkoxy carbonyl], which show photostability and activities of both leukotriene antagonism and inhibition of histamine release from mast cells, are prepd. A therapeutic or preventive drug contg. I as the active ingredient for the treatment of allergies or leukotriene and/or histamine-related diseases is claimed. Thus, 2-fluoro-4-[2-(4-methoxybenzyl)-2H-tetrazol-5-yl]benzoic acid was refluxed with SOCl2 in the presence of DMF in PhMe for 3 h and then condensed with 3-[2-(4-cyclobutyl-2-thiazolyl)ethynyl]aniline in the presence of Et3N, followed by treatment with anisole/CF3CO2H to give the title compd., ethynylthiazole contg. triazole deriv. (II). II in vitro showed IC50 5.7.times.10-10 M for inhibiting leukotriene D4-induced contraction of guinea pig's ileum and 9.3.times.10-9 M for inhibiting histamine release from rat's mast cells and in vivo inhibited leukotriene D4-induced contraction of guinea pig's air way with ID50 of 0.4 mg/kg p.o. An inhalant and capsule formulation contg. II were prepd.

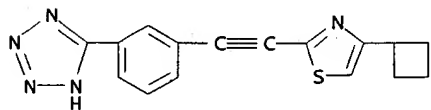
IT 211937-72-3P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of ethynylthiazole derivs. as leukotriene antagonists for

SEARCHED BY SUSAN HANLEY 305-4053

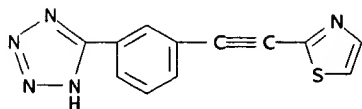
treatment of allergy and leukotriene and/histamine-related diseases)  
 RN 211937-72-3 HCAPLUS  
 CN 1H-Tetrazole, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA  
 INDEX NAME)



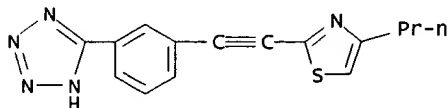
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 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic  
 preparation); THU (Therapeutic use); BIOL (Biological study);  
 PREP (Preparation); USES (Uses)  
 (prepn. of ethynylthiazole derivs. as leukotriene antagonists for  
 treatment of allergy and leukotriene and/or histamine-related diseases)  
 RN 211937-73-4 HCAPLUS



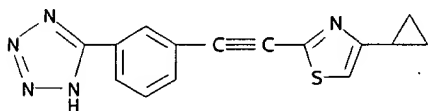
CN 1H-Tetrazole, 5-[3-(2-thiazolylethynyl)phenyl]- (9CI) (CA INDEX NAME)



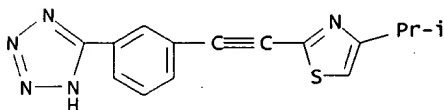
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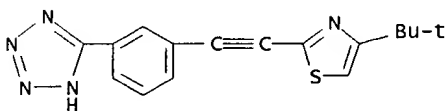
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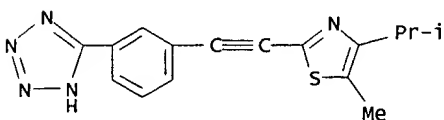
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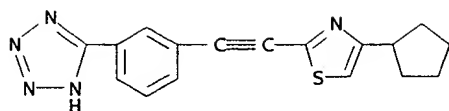
RN 211937-78-9 HCAPLUS  
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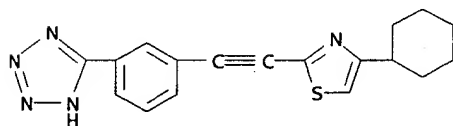
RN 211937-79-0 HCAPLUS  
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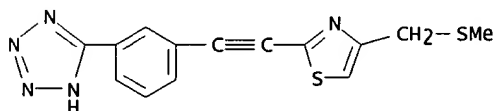
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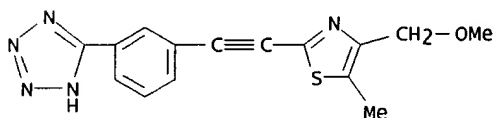
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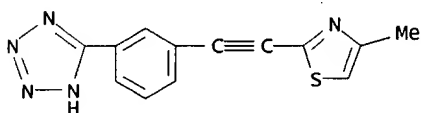
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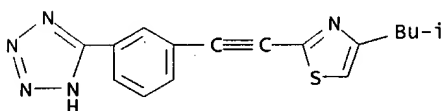
RN 211937-83-6 HCAPLUS  
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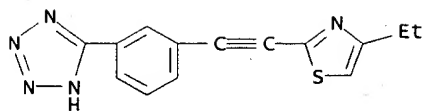
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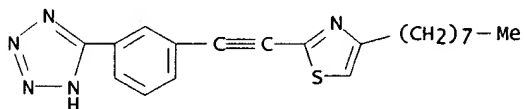
RN 211937-85-8 HCAPLUS  
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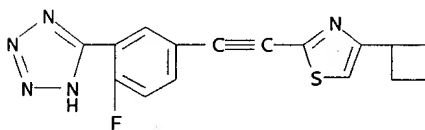
RN 211937-86-9 HCAPLUS  
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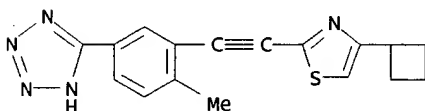
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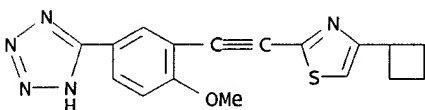
RN 211938-11-3 HCAPLUS  
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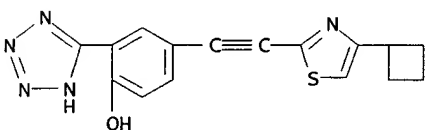
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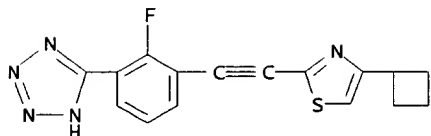
RN 211938-15-7 HCAPLUS  
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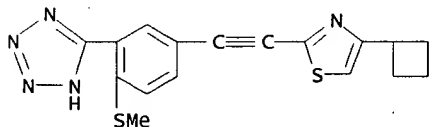
RN 211938-17-9 HCAPLUS  
CN Phenol, 4-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



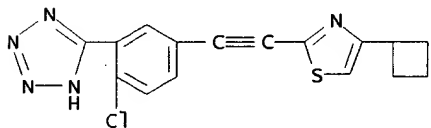
RN 211938-19-1 HCAPLUS  
CN 1H-Tetrazole, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-fluorophenyl]- (9CI) (CA INDEX NAME)



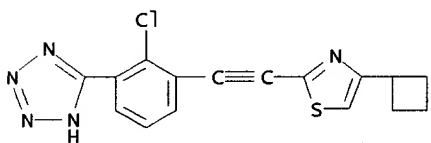
RN 211938-22-6 HCAPLUS  
CN 1H-Tetrazole, 5-[5-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-(methylthio)phenyl]- (9CI) (CA INDEX NAME)



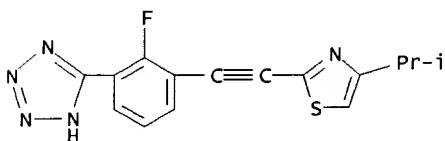
RN 211938-25-9 HCAPLUS  
CN 1H-Tetrazole, 5-[2-chloro-5-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



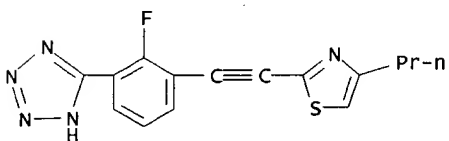
RN 211938-28-2 HCAPLUS  
CN 1H-Tetrazole, 5-[2-chloro-3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



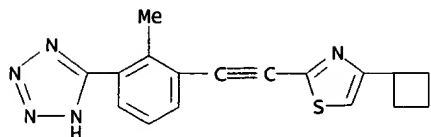
RN 211938-29-3 HCAPLUS  
CN 1H-Tetrazole, 5-[2-fluoro-3-[[4-(1-methylethyl)-2-thiazolyl]ethynyl]phenyl]- (9CI) (CA INDEX NAME)



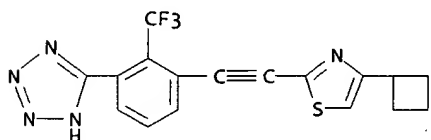
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CN 1H-Tetrazole, 5-[2-fluoro-3-[(4-propyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



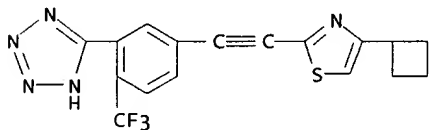
RN 211938-32-8 HCAPLUS  
 CN 1H-Tetrazole, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methylphenyl]-  
 (9CI) (CA INDEX NAME)



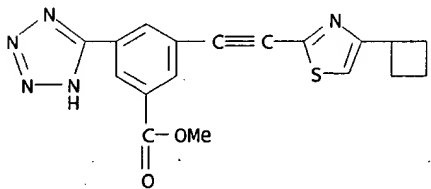
RN 211938-33-9 HCAPLUS  
 CN 1H-Tetrazole, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



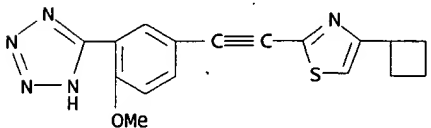
RN 211938-34-0 HCAPLUS  
 CN 1H-Tetrazole, 5-[5-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



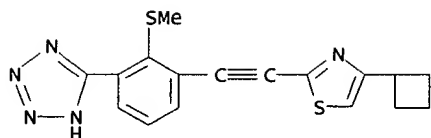
RN 211938-35-1 HCAPLUS  
 CN Benzoic acid, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-5-(1H-tetrazol-5-yl)-, methyl ester (9CI) (CA INDEX NAME)



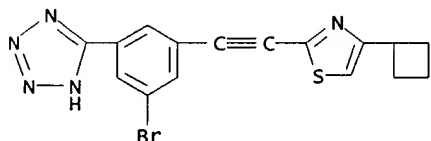
RN 211938-36-2 HCAPLUS  
 CN 1H-Tetrazole, 5-[5-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methoxyphenyl]-  
 (9CI) (CA INDEX NAME)



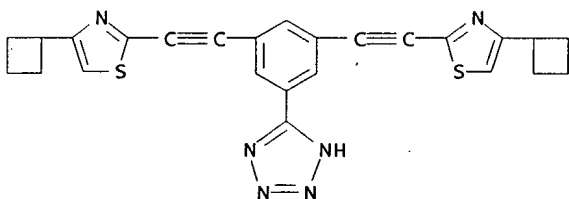
RN 211938-37-3 HCAPLUS  
 CN 1H-Tetrazole, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-(methylthio)phenyl]- (9CI) (CA INDEX NAME)



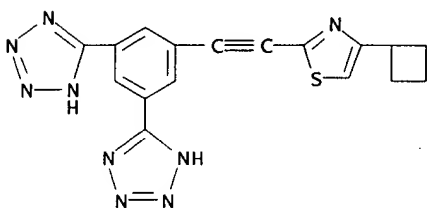
RN 211938-38-4 HCAPLUS  
CN 1H-Tetrazole, 5-[3-bromo-5-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



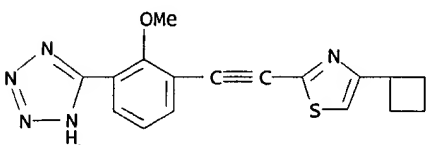
RN 211938-40-8 HCAPLUS  
CN 1H-Tetrazole, 5-[3,5-bis[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



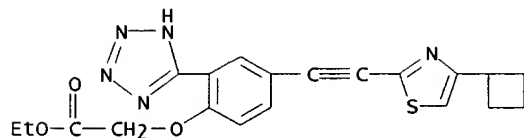
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CN 1H-Tetrazole, 5,5'-[5-[(4-cyclobutyl-2-thiazolyl)ethynyl]-1,3-phenylene]bis- (9CI) (CA INDEX NAME)



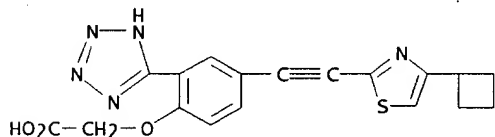
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CN 1H-Tetrazole, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methoxyphenyl]- (9CI) (CA INDEX NAME)



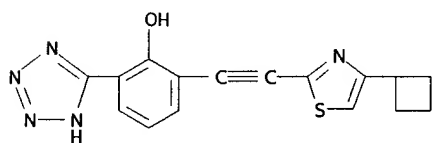
RN 211938-45-3 HCAPLUS  
CN Acetic acid, [4-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-(1H-tetrazol-5-yl)phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)



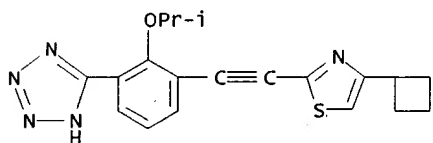
RN 211938-47-5 HCAPLUS  
 CN Acetic acid, [4-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-(1H-tetrazol-5-yl)phenoxy]- (9CI) (CA INDEX NAME)



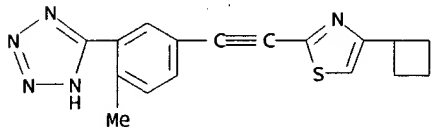
RN 211938-49-7 HCAPLUS  
 CN Phenol, 2-[(4-cyclobutyl-2-thiazolyl)ethynyl]-6-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



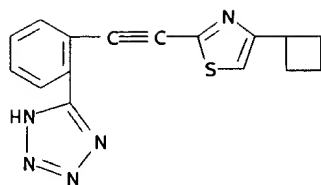
RN 211938-51-1 HCAPLUS  
 CN 1H-Tetrazole, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-(1-methylethoxy)phenyl]- (9CI) (CA INDEX NAME)



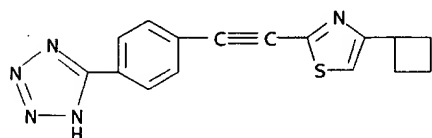
RN 211938-53-3 HCAPLUS  
 CN 1H-Tetrazole, 5-[5-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



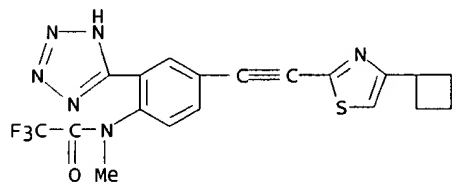
RN 211938-55-5 HCAPLUS  
 CN 1H-Tetrazole, 5-[2-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



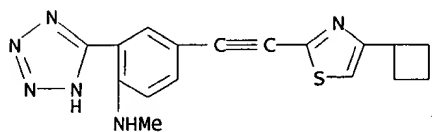
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CN 1H-Tetrazole, 5-[4-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



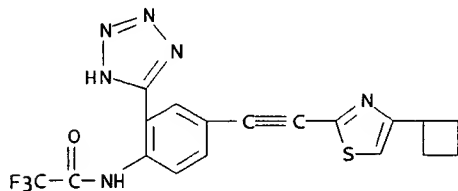
RN 211938-59-9 HCAPLUS  
CN Acetamide, N-[4-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-(1H-tetrazol-5-yl)phenyl]-2,2,2-trifluoro-N-methyl- (9CI) (CA INDEX NAME)



RN 211938-61-3 HCAPLUS  
CN Benzenamine, 4-[(4-cyclobutyl-2-thiazolyl)ethynyl]-N-methyl-2-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

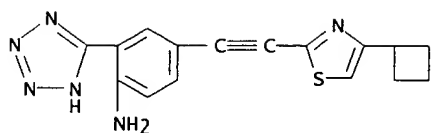


RN 211938-63-5 HCAPLUS  
CN Acetamide, N-[4-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-(1H-tetrazol-5-yl)phenyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

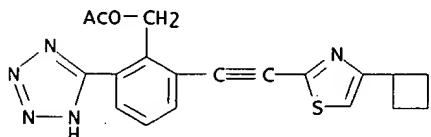


RN 211938-65-7 HCAPLUS  
CN Benzenamine, 4-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

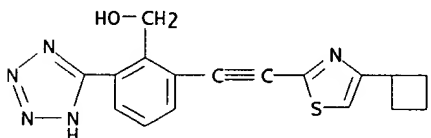




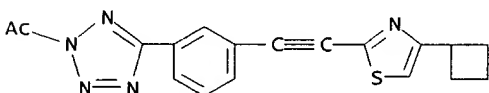
RN 211938-67-9 HCAPLUS  
CN Benzenemethanol, 2-[(4-cyclobutyl-2-thiazolyl)ethynyl]-6-(1H-tetrazol-5-yl)-, acetate (ester) (9CI) (CA INDEX NAME)



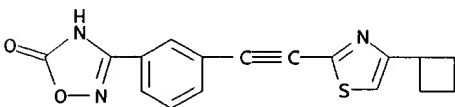
RN 211938-69-1 HCAPLUS  
CN Benzenemethanol, 2-[(4-cyclobutyl-2-thiazolyl)ethynyl]-6-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



RN 211938-72-6 HCAPLUS  
CN 2H-Tetrazole, 2-acetyl-5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)

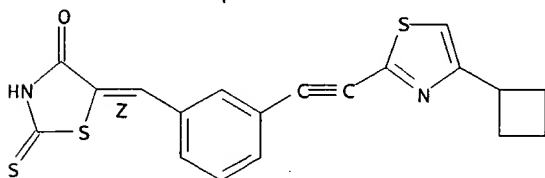


RN 211938-74-8 HCAPLUS  
CN 1,2,4-Oxadiazol-5(2H)-one, 3-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)

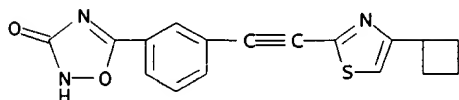


RN 211938-76-0 HCAPLUS  
CN 4-Thiazolidinone, 5-[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]methylene]-2-thioxo-, (5Z)- (9CI) (CA INDEX NAME)

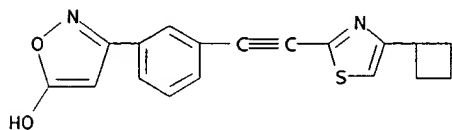
Double bond geometry as shown.



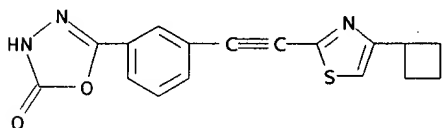
RN 211938-78-2 HCAPLUS  
 CN 1,2,4-Oxadiazol-3(2H)-one, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



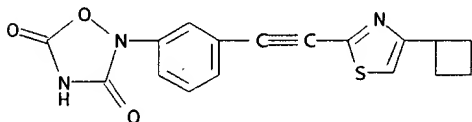
RN 211938-80-6 HCAPLUS  
 CN 5-Isoxazolol, 3-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



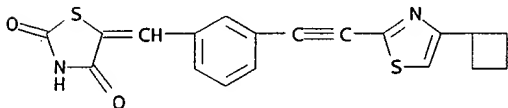
RN 211938-82-8 HCAPLUS  
 CN 1,3,4-Oxadiazol-2(3H)-one, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



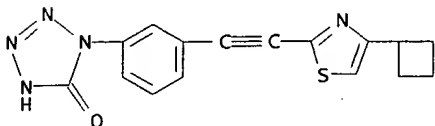
RN 211938-84-0 HCAPLUS  
 CN 1,2,4-Oxadiazolidine-3,5-dione, 2-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



RN 211938-86-2 HCAPLUS  
 CN 2,4-Thiazolidinedione, 5-[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]methylene]- (9CI) (CA INDEX NAME)

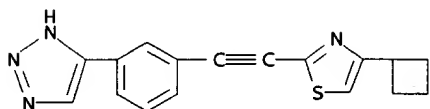


RN 211938-87-3 HCAPLUS  
 CN 5H-Tetrazol-5-one, 1-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-1,2-dihydro- (9CI) (CA INDEX NAME)

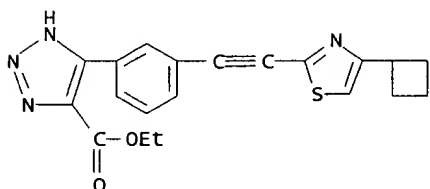


RN 211938-88-4 HCAPLUS

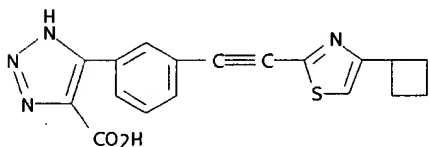
CN 1H-1,2,3-Triazole, 4-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI)  
(CA INDEX NAME)



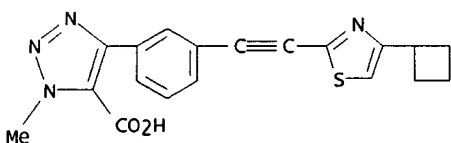
RN 211938-89-5 HCAPLUS  
CN 1H-1,2,3-Triazole-4-carboxylic acid, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)



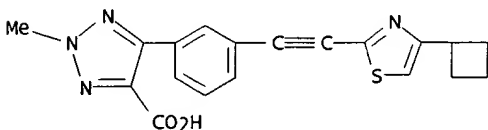
RN 211938-90-8 HCAPLUS  
CN 1H-1,2,3-Triazole-4-carboxylic acid, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



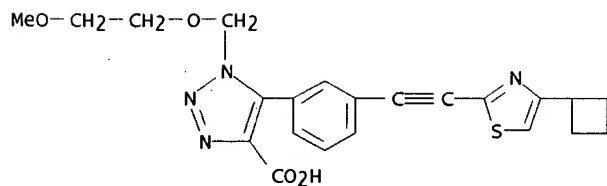
RN 211938-91-9 HCAPLUS  
CN 1H-1,2,3-Triazole-5-carboxylic acid, 4-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-1-methyl- (9CI) (CA INDEX NAME)



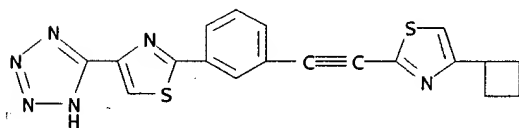
RN 211938-92-0 HCAPLUS  
CN 2H-1,2,3-Triazole-4-carboxylic acid, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-methyl- (9CI) (CA INDEX NAME)



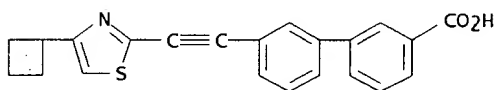
RN 211938-93-1 HCAPLUS  
CN 1H-1,2,3-Triazole-4-carboxylic acid, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-1-[(2-methoxyethoxy)methyl]- (9CI) (CA INDEX NAME)



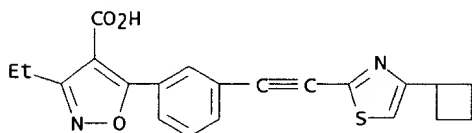
RN 211938-94-2 HCAPLUS  
CN 1H-Tetrazole, 5-[2-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)



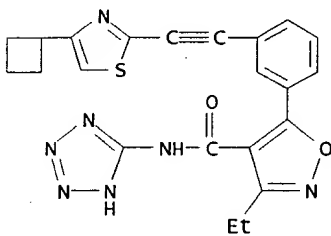
RN 211938-95-3 HCAPLUS  
CN [1,1'-Biphenyl]-3-carboxylic acid, 3'-[(4-cyclobutyl-2-thiazolyl)ethynyl]- (9CI) (CA INDEX NAME)



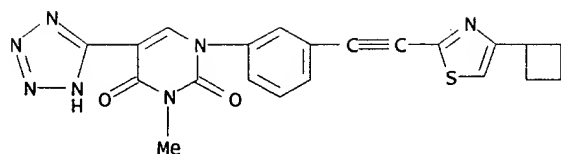
RN 211938-96-4 HCAPLUS  
CN 4-Isioxazolecarboxylic acid, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-ethyl- (9CI) (CA INDEX NAME)



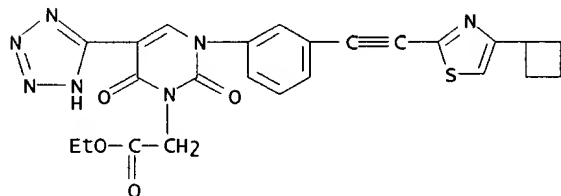
RN 211938-97-5 HCAPLUS  
CN 4-Isioxazolecarboxamide, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-ethyl-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)



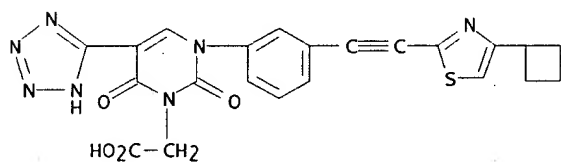
RN 211938-98-6 HCAPLUS  
CN 2,4(1H,3H)-Pyrimidinedione, 1-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-methyl-5-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



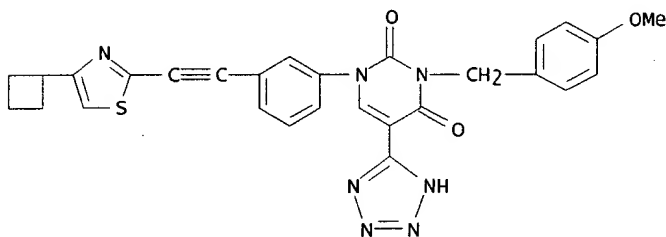
RN 211938-99-7 HCAPLUS  
 CN 1(2H)-Pyrimidineacetic acid, 3-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3,6-dihydro-2,6-dioxo-5-(1H-tetrazol-5-yl)-, ethyl ester (9CI) (CA INDEX NAME)



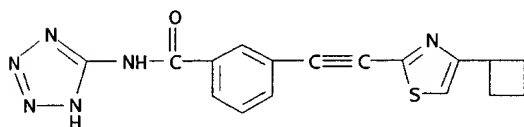
RN 211939-00-3 HCAPLUS  
 CN 1(2H)-Pyrimidineacetic acid, 3-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3,6-dihydro-2,6-dioxo-5-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



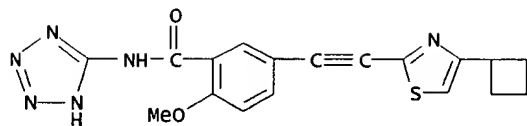
RN 211939-01-4 HCAPLUS  
 CN 2,4(1H,3H)-Pyrimidinedione, 1-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-[3-[(4-methoxyphenyl)methyl]-5-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



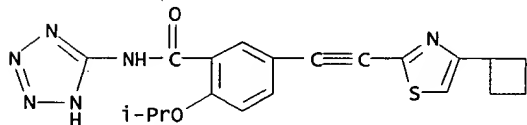
RN 211939-02-5 HCAPLUS  
 CN Benzamide, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)



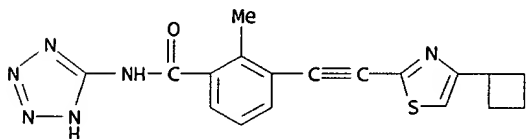
RN 211939-03-6 HCAPLUS  
 CN Benzamide, 5-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methoxy-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)



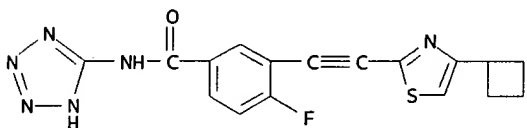
RN 211939-04-7 HCAPLUS  
CN Benzamide, 5-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-(1-methylethoxy)-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)



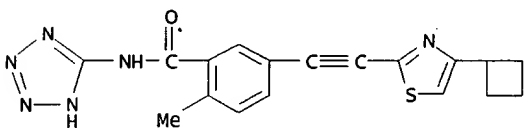
RN 211939-05-8 HCAPLUS  
CN Benzamide, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methyl-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)



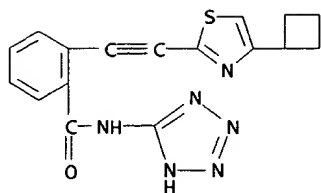
RN 211939-06-9 HCAPLUS  
CN Benzamide, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-4-fluoro-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)



RN 211939-07-0 HCAPLUS  
CN Benzamide, 5-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methyl-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)

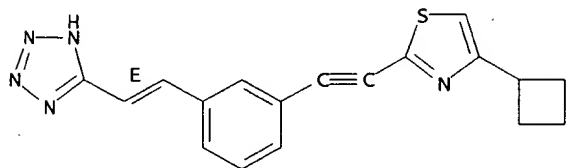


RN 211939-08-1 HCAPLUS  
CN Benzamide, 2-[(4-cyclobutyl-2-thiazolyl)ethynyl]-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)



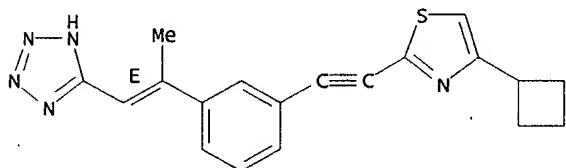
RN 211939-09-2 HCAPLUS  
CN 1H-Tetrazole, 5-[(1E)-2-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



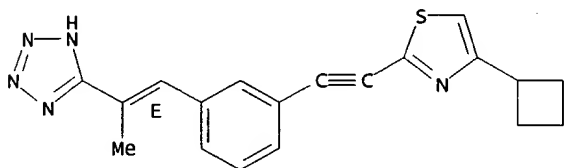
RN 211939-10-5 HCAPLUS  
CN 1H-Tetrazole, 5-[(1E)-2-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-1-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

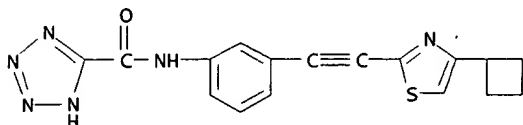


RN 211939-11-6 HCAPLUS  
CN 1H-Tetrazole, 5-[(1E)-2-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-1-methylethenyl]- (9CI) (CA INDEX NAME)

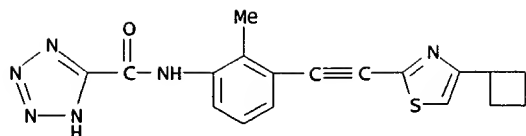
Double bond geometry as shown.



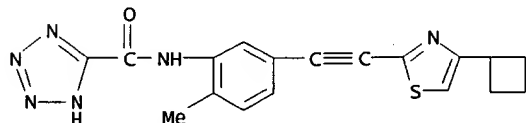
RN 211939-15-0 HCAPLUS  
CN 1H-Tetrazole-5-carboxamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



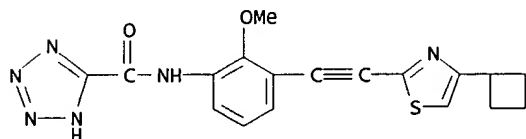
RN 211939-16-1 HCAPLUS  
CN 1H-Tetrazole-5-carboxamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



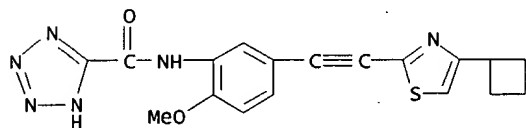
RN 211939-17-2 HCAPLUS  
 CN 1H-Tetrazole-5-carboxamide, N-[5-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



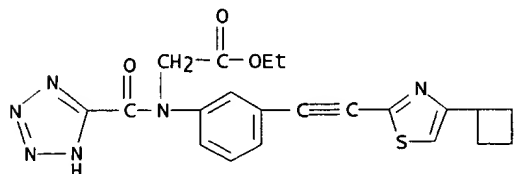
RN 211939-18-3 HCAPLUS  
 CN 1H-Tetrazole-5-carboxamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methoxyphenyl]- (9CI) (CA INDEX NAME)



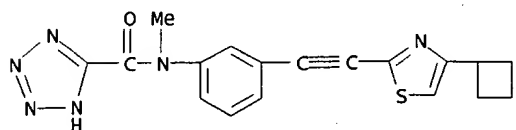
RN 211939-19-4 HCAPLUS  
 CN 1H-Tetrazole-5-carboxamide, N-[5-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methoxyphenyl]- (9CI) (CA INDEX NAME)



RN 211939-20-7 HCAPLUS  
 CN Glycine, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-N-(1H-tetrazol-5-ylcarbonyl)-, ethyl ester (9CI) (CA INDEX NAME)

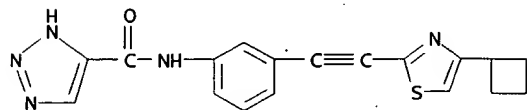


RN 211939-21-8 HCAPLUS  
 CN 1H-Tetrazole-5-carboxamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-N-methyl- (9CI) (CA INDEX NAME)

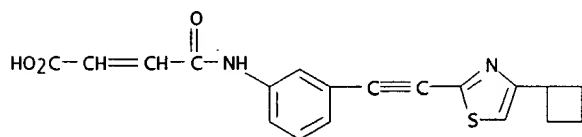




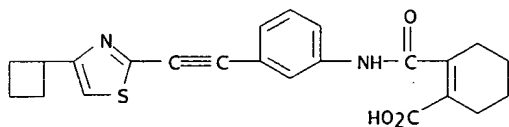
RN 211939-22-9 HCAPLUS  
 CN 1H-1,2,3-Triazole-4-carboxamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]- (9CI) (CA INDEX NAME)



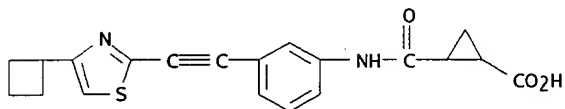
RN 211939-23-0 HCAPLUS  
 CN 2-Butenoic acid, 4-[[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]-4-oxo- (9CI) (CA INDEX NAME)



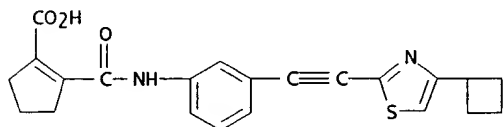
RN 211939-24-1 HCAPLUS  
 CN 1-cyclohexene-1-carboxylic acid, 2-[[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]carbonyl]- (9CI) (CA INDEX NAME)



RN 211939-25-2 HCAPLUS  
 CN Cyclopropanecarboxylic acid, 2-[[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]carbonyl]- (9CI) (CA INDEX NAME)

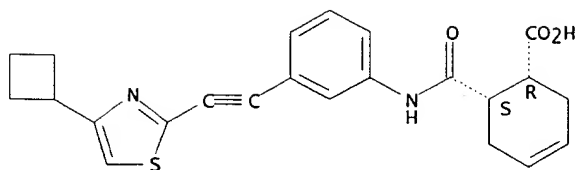


RN 211939-26-3 HCAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-[[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]carbonyl]- (9CI) (CA INDEX NAME)



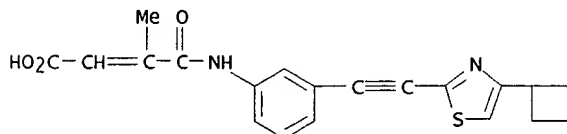
RN 211939-27-4 HCAPLUS  
 CN 3-Cyclohexene-1-carboxylic acid, 6-[[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]carbonyl]-, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



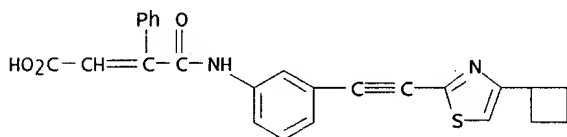
RN 211939-28-5 HCAPLUS

CN 2-Butenoic acid, 4-[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]-3-methyl-4-oxo- (9CI) (CA INDEX NAME)



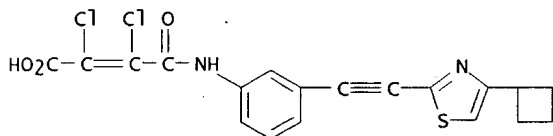
RN 211939-29-6 HCAPLUS

CN 2-Butenoic acid, 4-[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]-4-oxo-3-phenyl- (9CI) (CA INDEX NAME)



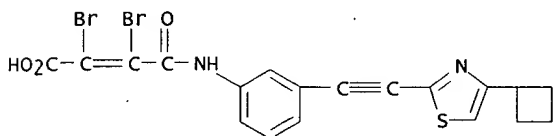
RN 211939-30-9 HCAPLUS

CN 2-Butenoic acid, 2,3-dichloro-4-[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]-4-oxo- (9CI) (CA INDEX NAME)



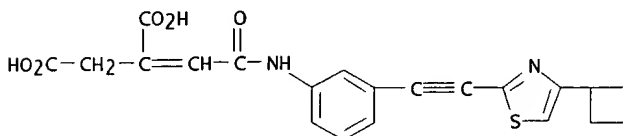
RN 211939-31-0 HCAPLUS

CN 2-Butenoic acid, 2,3-dibromo-4-[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]-4-oxo- (9CI) (CA INDEX NAME)



RN 211939-32-1 HCAPLUS

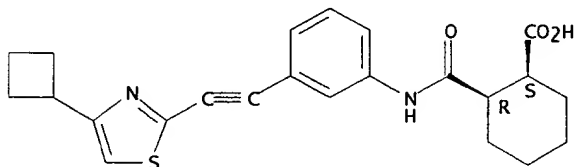
CN Butanedioic acid, [2-[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]-2-oxoethylidene]- (9CI) (CA INDEX NAME)



RN 211939-33-2 HCAPLUS

CN Cyclohexanecarboxylic acid, 2-[[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]carbonyl]-, (1R,2S)-rel- (9CI) (CA INDEX NAME)

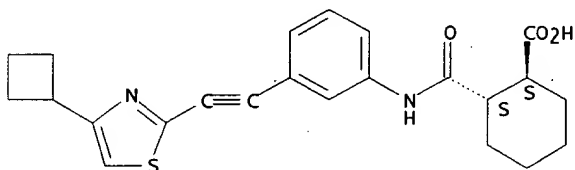
Relative stereochemistry.



RN 211939-34-3 HCAPLUS

CN Cyclohexanecarboxylic acid, 2-[[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]carbonyl]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

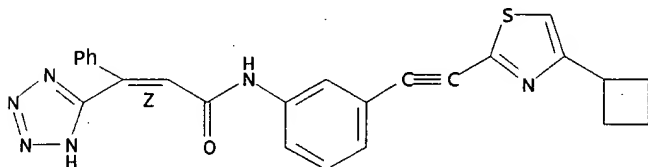
Relative stereochemistry.



RN 211939-36-5 HCAPLUS

CN 2-Propenamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-phenyl-3-(1H-tetrazol-5-yl)-, (2Z)- (9CI) (CA INDEX NAME)

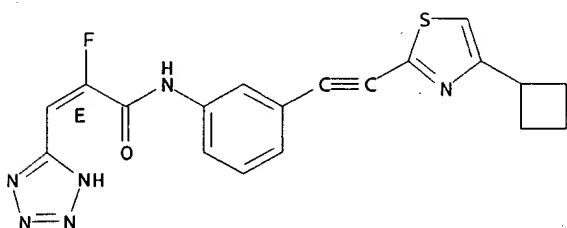
Double bond geometry as shown.



RN 211939-37-6 HCAPLUS

CN 2-Propenamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-fluoro-3-(1H-tetrazol-5-yl)-, (2E)- (9CI) (CA INDEX NAME)

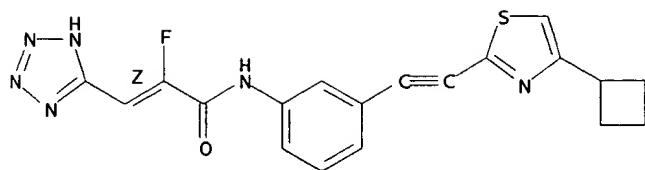
Double bond geometry as shown.



RN 211939-38-7 HCAPLUS

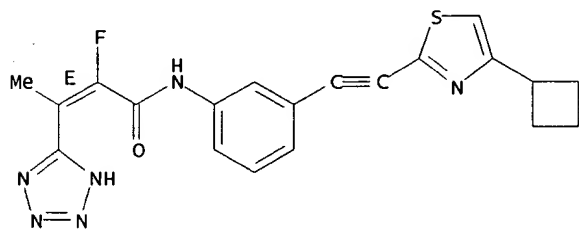
CN 2-Propenamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-fluoro-3-(1H-tetrazol-5-yl)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



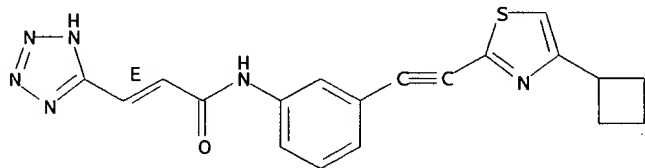
RN 211939-39-8 HCAPLUS  
 CN 2-Butenamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-fluoro-3-(1H-tetrazol-5-yl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

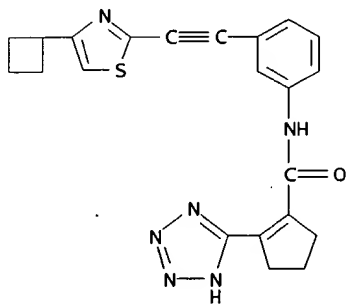


RN 211939-40-1 HCAPLUS  
 CN 2-Propenamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-(1H-tetrazol-5-yl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

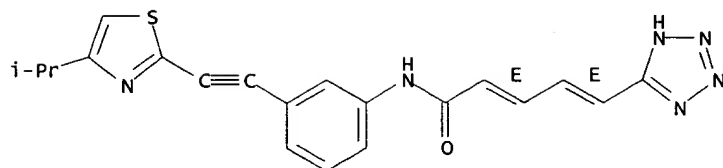


RN 211939-41-2 HCAPLUS  
 CN 1-Cyclopentene-1-carboxamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

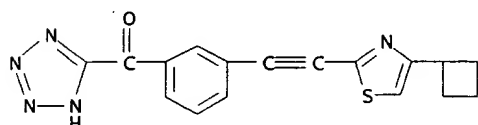


RN 211939-42-3 HCAPLUS  
 CN 2,4-Pentadienamide, N-[3-[[4-(1-methylethyl)-2-thiazolyl]ethynyl]phenyl]-5-(1H-tetrazol-5-yl)-, (2E,4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

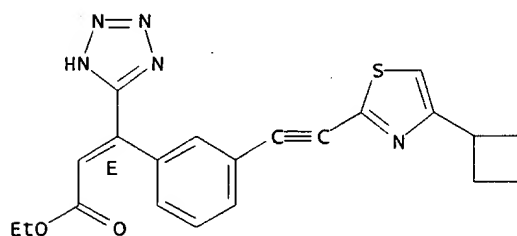


RN 211939-43-4 HCAPLUS  
 CN Methanone, [3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-1H-tetrazol-5-yl-  
 (9CI) (CA INDEX NAME)

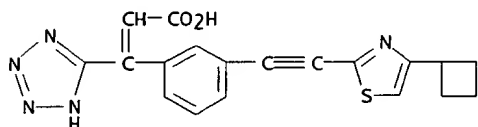


RN 211939-44-5 HCAPLUS  
 CN 2-Propenoic acid, 3-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-(1H-  
 tetrazol-5-yl)-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

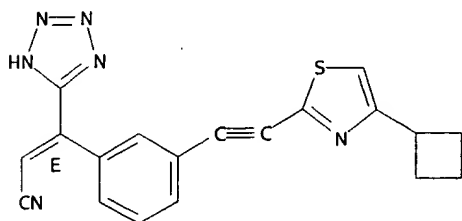


RN 211939-45-6 HCAPLUS  
 CN 2-Propenoic acid, 3-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-(1H-  
 tetrazol-5-yl)- (9CI) (CA INDEX NAME)

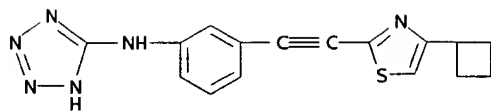


RN 211939-46-7 HCAPLUS  
 CN 2-Propenenitrile, 3-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-(1H-  
 tetrazol-5-yl)-, (2E)- (9CI) (CA INDEX NAME)

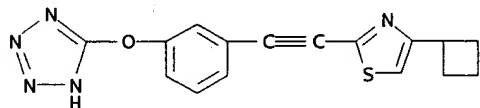
Double bond geometry as shown.



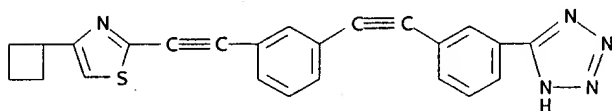
RN 211939-47-8 HCAPLUS  
 CN 1H-Tetrazol-5-amine, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-  
 (9CI) (CA INDEX NAME)



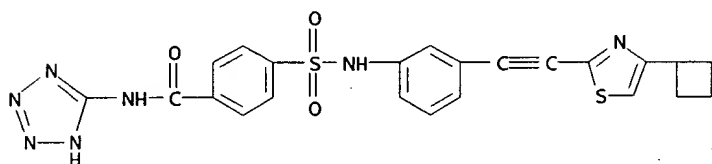
RN 211939-48-9 HCAPLUS  
CN 1H-Tetrazole, 5-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenoxy]- (9CI) (CA INDEX NAME)



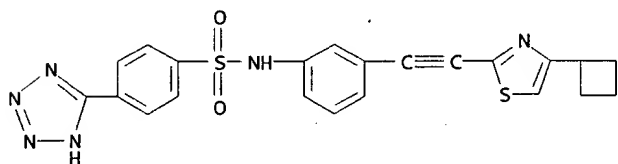
RN 211939-49-0 HCAPLUS  
CN 1H-Tetrazole, 5-[3-[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]ethynyl]phenyl]- (9CI) (CA INDEX NAME)



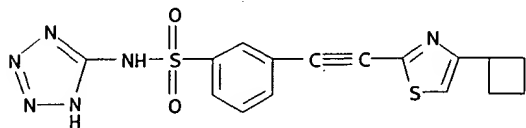
RN 211939-50-3 HCAPLUS  
CN Benzamide, 4-[[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]sulfonyl]-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)



RN 211939-51-4 HCAPLUS  
CN Benzenesulfonamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

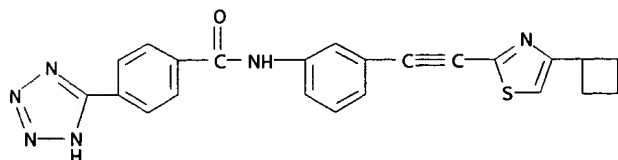


RN 211939-52-5 HCAPLUS  
CN Benzenesulfonamide, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)



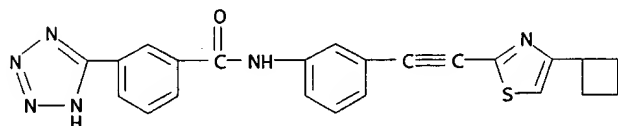
RN 211939-53-6 HCAPLUS

CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



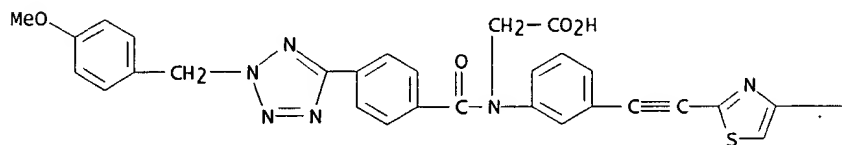
RN 211939-54-7 HCAPLUS

CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



RN 211939-55-8 HCAPLUS

CN Glycine, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-N-[4-[2-[(4-methoxyphenyl)methyl]-2H-tetrazol-5-yl]benzoyl]- (9CI) (CA INDEX NAME)



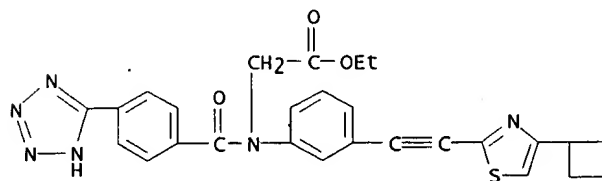
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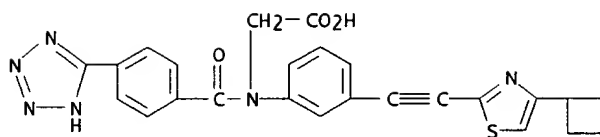
RN 211939-56-9 HCAPLUS

CN Glycine, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-N-[4-(1H-tetrazol-5-yl)benzoyl]-, ethyl ester (9CI) (CA INDEX NAME)

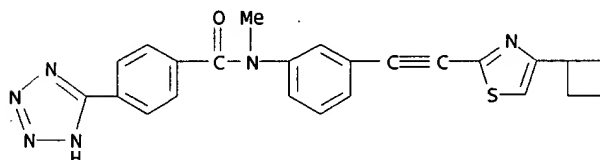


RN 211939-57-0 HCAPLUS

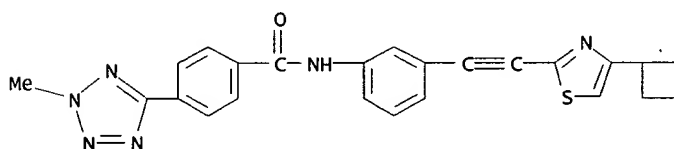
CN Glycine, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-N-[4-(1H-tetrazol-5-yl)benzoyl]- (9CI) (CA INDEX NAME)



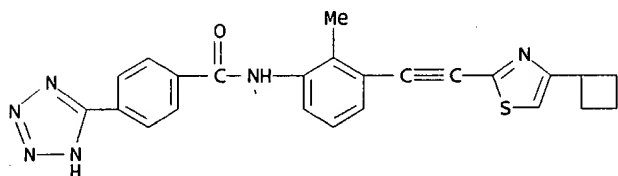
RN 211939-58-1 HCAPLUS  
CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-N-methyl-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



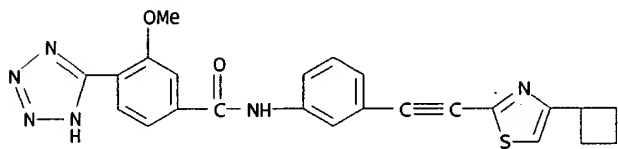
RN 211939-59-2 HCAPLUS  
CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-4-(2-methyl-2H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



RN 211939-61-6 HCAPLUS  
CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methylphenyl]-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

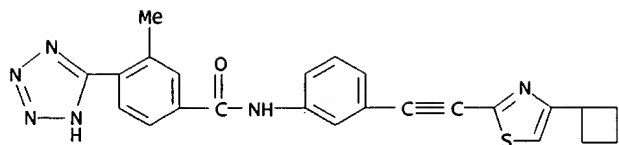


RN 211939-62-7 HCAPLUS  
CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-methoxy-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

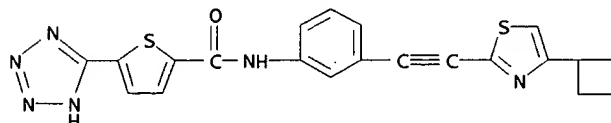


RN 211939-64-9 HCAPLUS  
CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-methyl-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

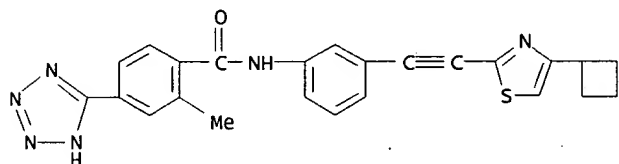




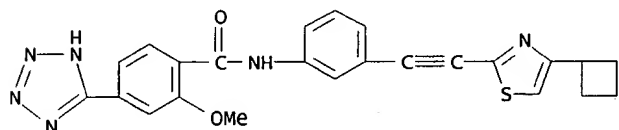
RN 211939-66-1 HCAPLUS  
 CN 2-Thiophenecarboxamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-5-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



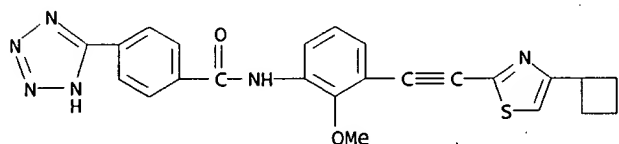
RN 211939-68-3 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-methyl-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



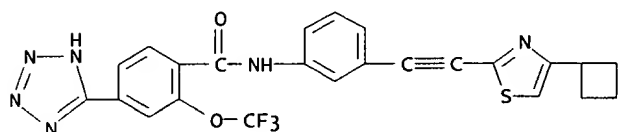
RN 211939-69-4 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-methoxy-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



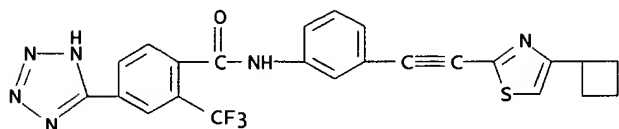
RN 211939-70-7 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-methoxyphenyl]-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



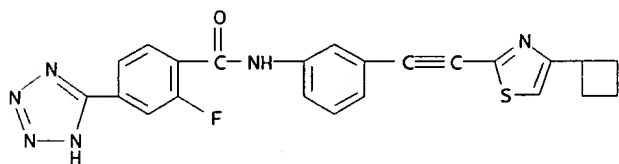
RN 211939-71-8 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-4-(1H-tetrazol-5-yl)-2-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



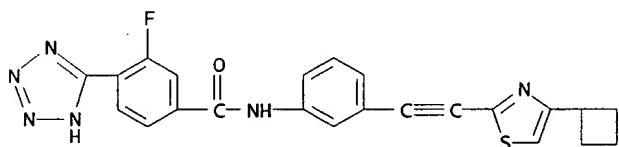
RN 211939-72-9 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-4-(1H-tetrazol-5-yl)-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



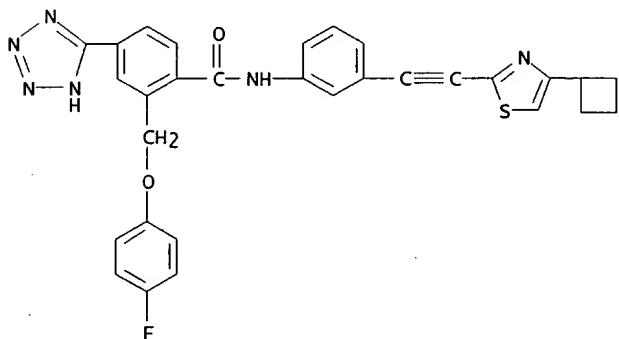
RN 211939-73-0 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-fluoro-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



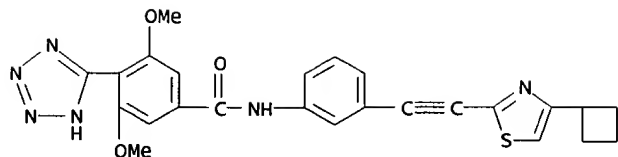
RN 211939-74-1 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-fluoro-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



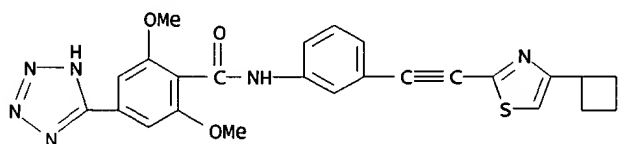
RN 211939-75-2 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-[(4-fluorophenoxy)methyl]-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



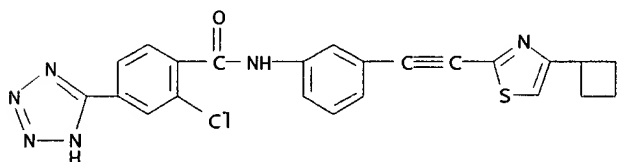
RN 211939-76-3 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3,5-dimethoxy-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



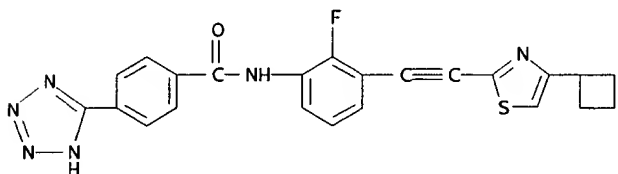
RN 211939-77-4 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2,6-dimethoxy-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



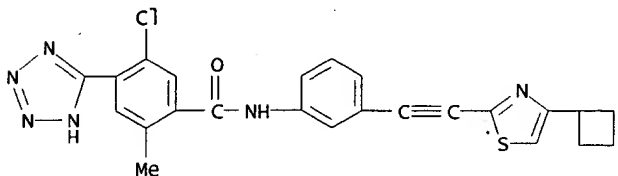
RN 211939-78-5 HCAPLUS  
 CN Benzamide, 2-chloro-N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



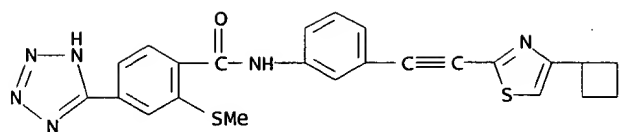
RN 211939-79-6 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-fluorophenyl]-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



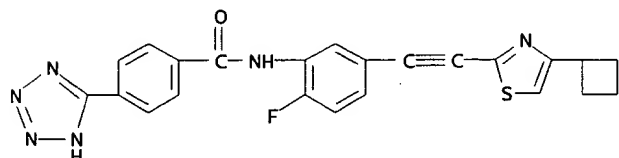
RN 211939-80-9 HCAPLUS  
 CN Benzamide, 5-chloro-N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-methyl-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



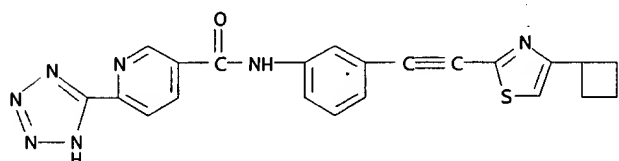
RN 211939-81-0 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-(methylthio)-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



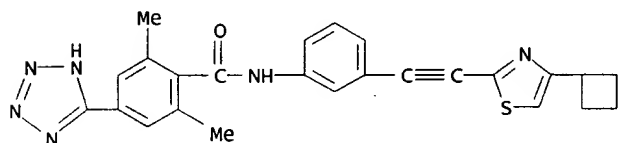
RN 211939-82-1 HCAPLUS  
 CN Benzamide, N-[5-[[4-(4-cyclobutyl-2-thiazolyl)ethynyl]-2-fluorophenyl]-4-(1H-tetrazol-5-yl)]- (9CI) (CA INDEX NAME)



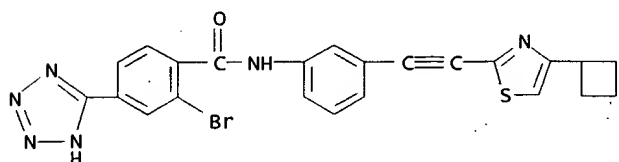
RN 211939-83-2 HCAPLUS  
 CN 3-Pyridinecarboxamide, N-[3-[[4-(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-6-(1H-tetrazol-5-yl)]- (9CI) (CA INDEX NAME)



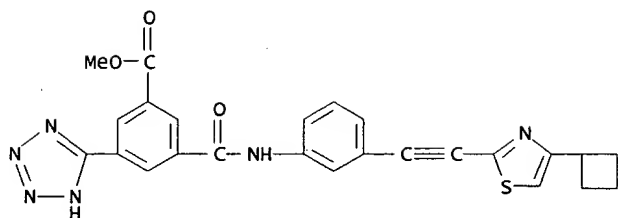
RN 211939-84-3 HCAPLUS  
 CN Benzamide, N-[3-[[4-(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2,6-dimethyl-4-(1H-tetrazol-5-yl)]- (9CI) (CA INDEX NAME)



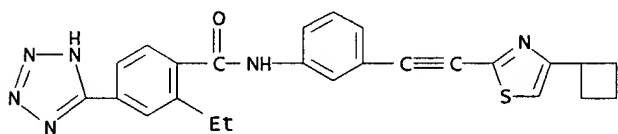
RN 211939-85-4 HCAPLUS  
 CN Benzamide, 2-bromo-N-[3-[[4-(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-4-(1H-tetrazol-5-yl)]- (9CI) (CA INDEX NAME)



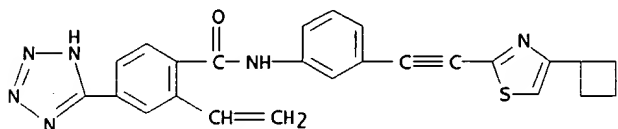
RN 211939-86-5 HCAPLUS  
 CN Benzoic acid, 3-[[[3-[[4-(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]amino]carbonyl]-5-(1H-tetrazol-5-yl)]-, methyl ester (9CI) (CA INDEX NAME)



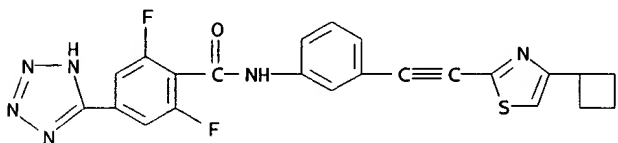
RN 211939-87-6 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-ethyl-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



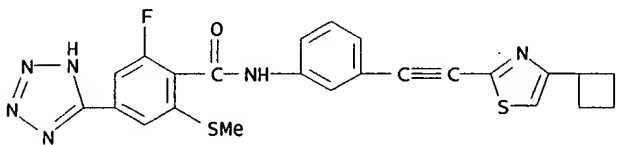
RN 211939-88-7 HCAPLUS  
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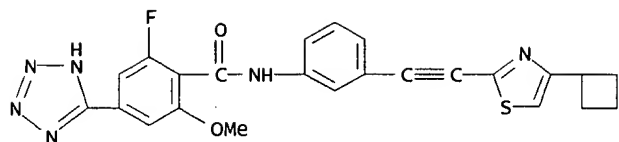
RN 211939-89-8 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2,6-difluoro-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



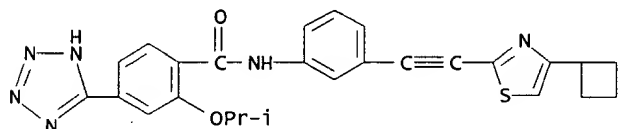
RN 211939-90-1 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-fluoro-6-(methylthio)-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



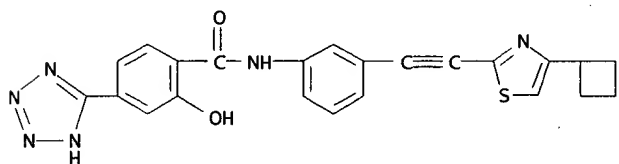
RN 211939-91-2 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-fluoro-6-methoxy-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



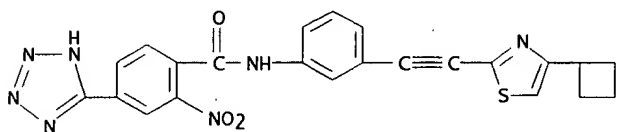
RN 211939-92-3 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-(1-methylethoxy)-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



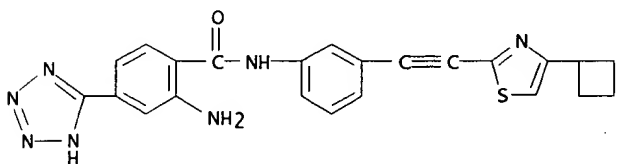
RN 211939-93-4 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-hydroxy-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



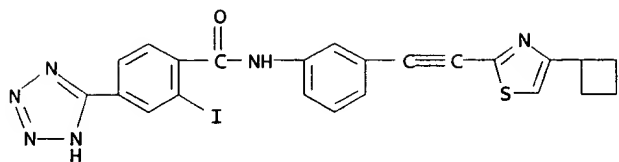
RN 211939-94-5 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-nitro-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



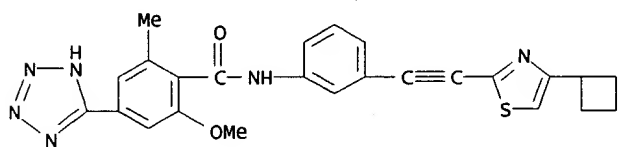
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 CN Benzamide, 2-amino-N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



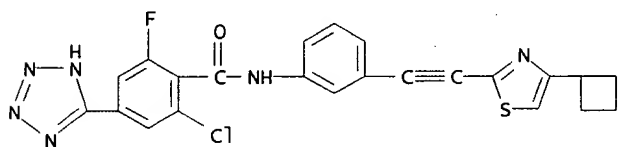
RN 211939-96-7 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-iodo-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



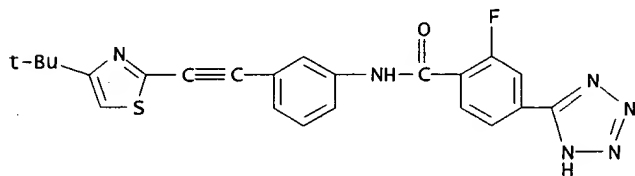
RN 211939-97-8 HCAPLUS  
 CN Benzamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-2-methoxy-6-methyl-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



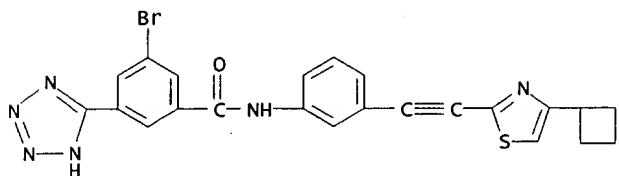
RN 211939-98-9 HCAPLUS  
 CN Benzamide, 2-chloro-N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-6-fluoro-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



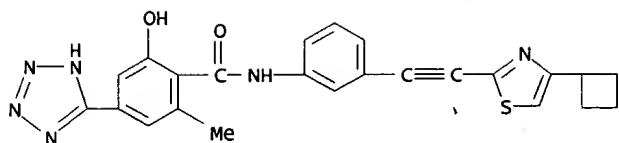
RN 211939-99-0 HCAPLUS  
 CN Benzamide, N-[3-[[4-(1,1-dimethylethyl)-2-thiazolyl]ethynyl]phenyl]-2-fluoro-4-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



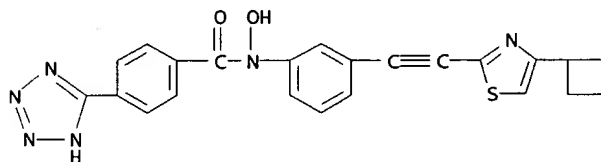
RN 211940-00-0 HCAPLUS  
 CN Benzamide, 3-bromo-N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-5-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



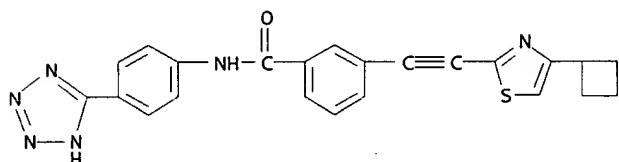
RN 211940-01-1 HCAPLUS  
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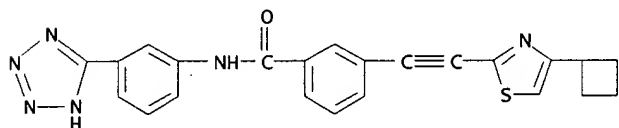
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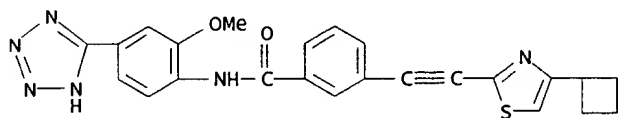
RN 211940-03-3 HCAPLUS  
 CN Benzamide, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-N-[4-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)



RN 211940-04-4 HCAPLUS  
 CN Benzamide, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-N-[3-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

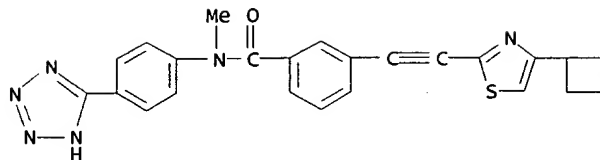


RN 211940-05-5 HCAPLUS  
 CN Benzamide, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-N-[2-methoxy-4-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

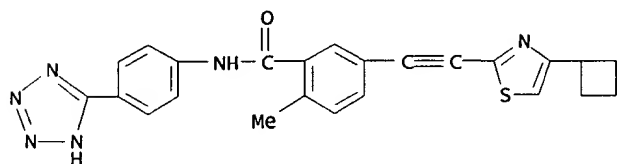


RN 211940-06-6 HCAPLUS  
 CN Benzamide, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-N-methyl-N-[4-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

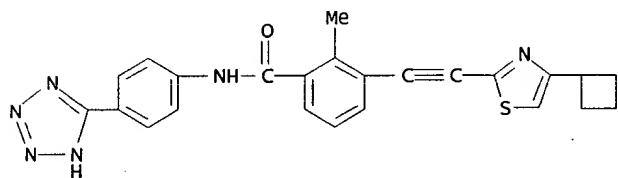




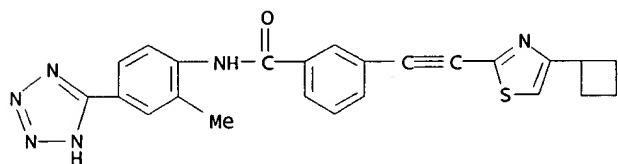
RN 211940-07-7 HCAPLUS  
 CN Benzamide, 5-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methyl-N-[4-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)



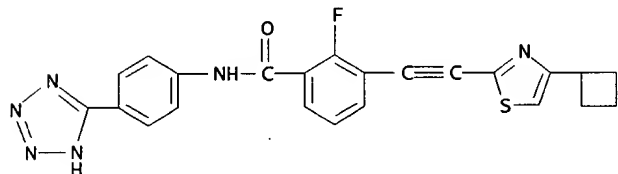
RN 211940-08-8 HCAPLUS  
 CN Benzamide, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-methyl-N-[4-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)



RN 211940-09-9 HCAPLUS  
 CN Benzamide, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-N-[2-methyl-4-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

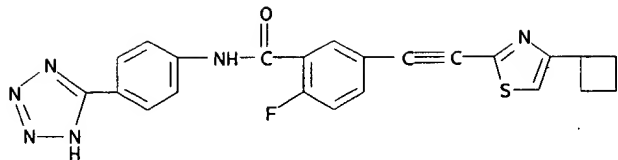


RN 211940-10-2 HCAPLUS  
 CN Benzamide, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-fluoro-N-[4-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

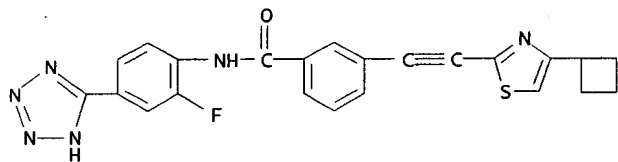


RN 211940-11-3 HCAPLUS  
 CN Benzamide, 5-[(4-cyclobutyl-2-thiazolyl)ethynyl]-2-fluoro-N-[4-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

CHOI 09/387,135



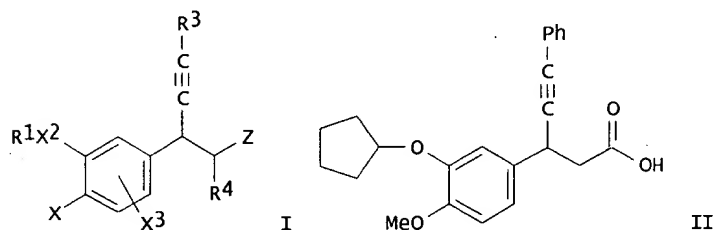
RN 211940-12-4 HCAPLUS  
CN Benzamide, 3-[(4-cyclobutyl-2-thiazolyl)ethynyl]-N-[2-fluoro-4-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)



=&gt; d bib abs hitstr 154 4

L54 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1997:224040 HCAPLUS  
 DN 126:211918  
 TI Substituted pent-4-ynoic acids useful for inhibiting production of tumor necrosis factor (TNF)  
 IN Christensen, Siegfried B., IV; Karpinski, Joseph M.; Frazee, James S.  
 PA Smithkline Beecham Corporation, USA; Christensen, Siegfried B., IV.; Karpinski, Joseph M.; Frazee, James S.  
 SO PCT Int. Appl., 77 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9703945	A1	19970206	WO 1996-US11613	19960712
	W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9664903	A1	19970218	AU 1996-64903	19960712
	EP 827495	A1	19980311	EP 1996-924459	19960712
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI				
	US 6037367	A	20000314	US 1998-716359	19980914
PRAI	US 1995-1196		19950714		
	US 1996-16717		19960502		
	WO 1996-US11613		19960712		
OS	MARPAT 126:211918				
GI					



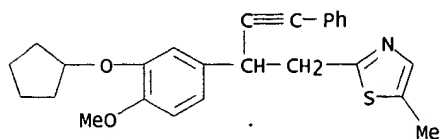
AB Title compds. I [R1 = wide variety of sidechains contg. esters, amides, ethers, and a variety of functional groups; X = YR2, F, (di)(alkyl)amino, formylamino; Y = O, S, SO, SO2; X2 = O, NH, (fluoro)(alkyl)imino; X3 = H, X; Z = acyl, CO2H and derivs., NH2 and derivs., certain (un)substituted azoles; R2 = Me, Et, or their halo derivs.; R3 = H, alkyl, Ph, phenylalkyl, pyrimidyl(alkyl), imidazolyl(alkyl); R4 = H, acyl, CO2H or esters, CONH2 or derivs., OH or SH or derivs.] and their pharmaceutically acceptable salts are claimed, and approx. 140 examples were prepd. As inhibitors of the enzyme PDE IV (no data), I are useful for treatment of allergy, inflammation, and asthma. As inhibitors of TNF (tumor necrosis factor) prodn. in mammals (no data), I are also useful for treating viral infections (including HIV) and yeast or fungal infections which are sensitive to TNF. For instance, the acid II was prepd. in 3 steps. Specifically, 2,2-dimethyl-1,3-dioxane-4,6-dione was condensed with 3-(cyclopentyloxy)-4-methoxybenzaldehyde to give the 5-benzylidene deriv. (93%), which underwent alkylation with PhC.tplbond.CLi (84%), followed by hydrolysis with aq. HCl in dioxane, and thermal decarboxylation in ACNMe2 at 135.degree. (82%), to give II.

IT 188009-39-4P 188009-40-7P 188009-51-0P  
 188009-53-2P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of substituted pentynoic acids useful as inhibitors of TNF prodn.)

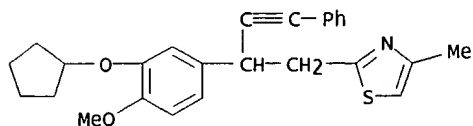
SEARCHED BY SUSAN HANLEY 305-4053

Page 41

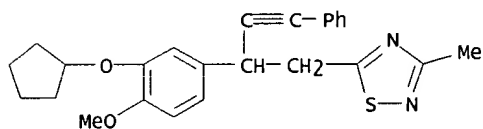
RN 188009-39-4 HCAPLUS  
 CN Thiazole, 2-[2-[3-(cyclopentyloxy)-4-methoxyphenyl]-4-phenyl-3-butynyl]-5-methyl- (9CI) (CA INDEX NAME)



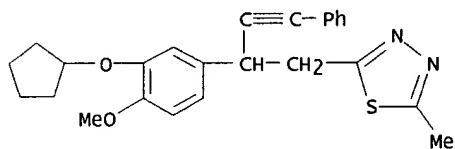
RN 188009-40-7 HCAPLUS  
 CN Thiazole, 2-[2-[3-(cyclopentyloxy)-4-methoxyphenyl]-4-phenyl-3-butynyl]-4-methyl- (9CI) (CA INDEX NAME)



RN 188009-51-0 HCAPLUS  
 CN 1,2,4-Thiadiazole, 5-[2-[3-(cyclopentyloxy)-4-methoxyphenyl]-4-phenyl-3-butynyl]-3-methyl- (9CI) (CA INDEX NAME)



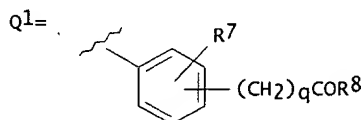
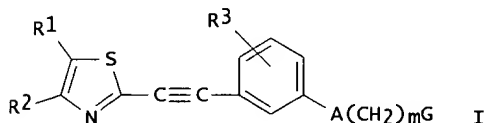
RN 188009-53-2 HCAPLUS  
 CN 1,3,4-Thiadiazole, 2-[2-[3-(cyclopentyloxy)-4-methoxyphenyl]-4-phenyl-3-butynyl]-5-methyl- (9CI) (CA INDEX NAME)



=&gt; d bib abs hitstr 154 5

L54 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1996:746320 HCAPLUS  
 DN 126:18869  
 TI Preparation of (arylethynyl)thiazole derivatives as leukotriene antagonists.  
 IN Nakayama, Atsushi; Machinaga, Nobuo; Yamaguchi, Hitoshi; Takeda, Toshiyuki; Haruta, Makoto; Ogasawara, Tomomi; Matsumura, Manabu  
 PA Daiichi Pharmaceutical Co., Ltd., Japan; Nakayama, Atsushi; Machinaga, Nobuo; Yamaguchi, Hitoshi; Takeda, Toshiyuki; Haruta, Makoto; Ogasawara, Tomomi; Matsumura, Manabu  
 SO PCT Int. Appl., 80 pp  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9633181	A1	19961024	WO 1996-JP1079	19960419
	W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9653474	A1	19961107	AU 1996-53474	19960419
	JP 11506425	T2	19990608	JP 1996-531628	19960419
PRAI	JP 1995-97002		19950421		
	WO 1996-JP1079		19960419		
OS	MARPAT 126:18869				
GI					



AB Title compds. [I; R1, R2 = H, halo, (substituted) alkyl, cycloalkyl; R1R2 = atoms to form a ring; R3 = H, OH, halo, (substituted) alkyl; A = NHCO, CONH, NHSO2; m = 0-3; G = CR4R5(CH2)nCOR6, Q1; n R4, R5 = H, (substituted) alkyl; R4R5 = atoms to form a ring; n = 0, 1; R6 = OH, (substituted) alkoxy group; R7 = H, OH, halo, (substituted) alkyl alkoxy, cyano, NO2, (substituted) alkoxy carbonyl; q = 0, 1; and R8 = OH, (substituted) alkoxy], were prepd. Thus, 3-[2-(4-cyclobutyl-2-thiazolyl)ethynyl]aniline (prepn. given) was refluxed with homophthalic anhydride in PhMe to give 2-[2-[3-[2-(4-cyclobutyl-2-thiazolyl)ethynyl]phenylamino]-2-oxoethyl]benzoic acid. The latter antagonized LTD4 in guinea pig ileum with IC50 = 3.4 .times. 10-10 M.

IT 184154-26-5P 184154-28-7P 184154-30-1P  
 184154-32-3P 184154-33-4P 184154-35-6P  
 184154-52-7P 184154-53-8P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of arylethynylthiazole derivs. as leukotriene antagonists)

RN 184154-26-5 HCAPLUS  
 CN Pentanamide, N-[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]phenyl]-3-ethyl-3-methyl- (9CI) (CA INDEX NAME)

L31 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:701075 CAPLUS

DOCUMENT NUMBER: 121:301075

TITLE: Preparation of phosphonic acid derivatives useful for medically treating hyperlipemia

INVENTOR(S): Yoshida, Ichirou; Ikuta, Hironori; Fukuda, Yoshio; Eguchi, Yoshihito; Kaino, Makoto; Tagami, Katsuya; Kobayashi, Naoki; Hayashi, Kenji; Hiyoshi, Hironobu; et al.

PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan

SOURCE: PCT Int. Appl., 363 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

INT. PATENT CLASSIF.:

MAIN: C07F009-38

SECONDARY: A61K031-66; C07F009-40; C07F009-59; C07F009-58;  
C07F009-655; C07F009-6506; C07F009-6553; C07F009-572;  
C07F009-6558; C07F009-653; C07F009-6512;

C07F009-6533;

C07F009-6539; C07F009-6541; C07F9 -6503; C07F9  
-6509; C07F9 -6574; C07F9 -62; C07F9 -60

CLASSIFICATION: 29-7 (Organometallic and Organometalloidal Compounds)  
Section cross-reference(s): 1

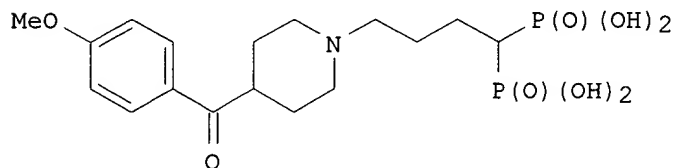
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9420508	A1	19940915	WO 1994-JP354	19940304
W: AU, CA, CN, FI, HU, JP, KR, NO, NZ, RU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9461564	A1	19940926	AU 1994-61564	19940304
EP 688325	A1	19951227	EP 1994-908498	19940304
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
HU 72307	A2	19960429	HU 1995-1944	19940304
JP 08508245	T2	19960903	JP 1994-519819	19940304
ZA 9401575	A	19941013	ZA 1994-1575	19940307
US 5719303	A	19980217	US 1995-530311	19950906
PRIORITY APPLN. INFO.:			JP 1993-46389	19930308
			WO 1994-JP354	19940304

OTHER SOURCE(S): MARPAT 121:301075

GRAPHIC IMAGE:



ABSTRACT:

533 Phosphonic acid derivs. RACRBR1P(O) (OR2) (OR3), e.g., I, or their pharmacol. acceptable salts, useful for medically treating hyperlipemia, were prepd. The compds. of the present invention act as effective squalene synthetase inhibitors (test data given).

SUPPL. TERM: phosphonic acid prepn hyperlipemia; squalene synthetase inhibitor phosphonic acid

INDEX TERM: Lipids, biological studies

ROLE: BAC (Biological activity or effector, except adverse);

THU (Therapeutic use); BIOL (Biological study); USES (Uses) (metabolic disorders, hyperlipidemia, prepn. of phosphonic acid derivs. useful for medically treating hyperlipemia)

INDEX TERM: 159269-80-4P 159269-81-5P 159269-82-6P 159269-85-9P 159269-90-6P 159269-92-8P 159269-96-2P 159270-00-5P

ROLE: BAC (Biological activity or effector, except adverse);

RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of phosphonic acid derivs. useful for medically treating hyperlipemia)

INDEX TERM: 150230-59-4P 150230-60-7P 159269-83-7P 159269-84-8P 159269-86-0P 159269-87-1P 159269-88-2P 159269-89-3P 159269-91-7P 159269-93-9P 159269-94-0P 159269-95-1P 159269-97-3P 159269-98-4P 159269-99-5P 159270-01-6P 159270-02-7P 159270-03-8P 159270-04-9P 159270-05-0P 159270-06-1P 159270-07-2P 159270-08-3P 159270-09-4P 159270-10-7P 159270-11-8P 159270-12-9P 159270-13-0P 159270-14-1P 159270-15-2P 159270-16-3P 159270-17-4P 159270-18-5P 159270-19-6P 159270-20-9P 159270-21-0P 159270-22-1P 159270-23-2P 159270-24-3P 159270-25-4P 159270-26-5P 159270-27-6P 159270-28-7P 159270-29-8P 159270-30-1P 159270-31-2P 159270-32-3P 159270-33-4P 159270-34-5P 159270-35-6P 159270-36-7P 159270-37-8P 159270-38-9P 159270-39-0P 159270-40-3P 159270-41-4P 159270-42-5P 159270-43-6P 159270-44-7P 159270-45-8P 159270-46-9P 159270-47-0P 159270-48-1P 159270-49-2P 159270-50-5P 159270-51-6P 159270-52-7P 159270-53-8P 159270-54-9P 159270-55-0P 159270-56-1P 159270-57-2P 159270-58-3P 159270-59-4P 159270-60-7P 159270-61-8P 159270-62-9P 159270-63-0P 159270-64-1P 159270-65-2P 159270-66-3P 159270-67-4P 159270-68-5P 159270-69-6P 159270-70-9P 159270-71-0P 159270-72-1P 159270-73-2P 159270-74-3P 159270-75-4P 159270-76-5P 159270-77-6P 159270-78-7P 159270-79-8P 159270-80-1P 159270-81-2P 159270-82-3P 159270-83-4P 159270-84-5P 159270-85-6P 159270-86-7P 159270-87-8P 159270-88-9P 159270-89-0P 159270-90-3P 159270-91-4P 159270-92-5P 159270-93-6P 159270-94-7P 159270-95-8P 159270-96-9P 159270-97-0P 159270-98-1P 159270-99-2P 159271-00-8P

159271-01-9P	159271-02-0P	159271-03-1P	159271-04-2P
159271-05-3P	159271-06-4P	159271-07-5P	159271-08-6P
159271-09-7P	159271-10-0P	159271-11-1P	159271-12-2P
159271-13-3P	159271-14-4P	159271-15-5P	159271-16-6P
159271-17-7P	159271-18-8P	159271-19-9P	159271-20-2P
159271-21-3P	159271-22-4P	159271-23-5P	159271-24-6P
159271-25-7P	159271-26-8P	159271-27-9P	159271-28-0P
159271-29-1P	159271-30-4P	159271-31-5P	159271-32-6P
159271-33-7P	159271-34-8P	159271-35-9P	159271-36-0P
159271-37-1P	159271-38-2P	159271-39-3P	159271-40-6P
159271-41-7P	159271-42-8P	159271-43-9P	159271-44-0P
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159271-49-5P	159271-50-8P	159271-51-9P	159271-52-0P
159271-53-1P	159271-54-2P	159271-55-3P	159271-56-4P
159271-57-5P	159271-58-6P	159271-59-7P	159271-60-0P
159271-61-1P	159271-62-2P	159271-63-3P	159271-64-4P
159271-65-5P	159271-66-6P	159271-67-7P	159271-68-8P
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159271-73-5P	159271-74-6P	159271-75-7P	159271-76-8P
159271-77-9P	159271-78-0P	159271-79-1P	159271-80-4P
159271-81-5P	159271-82-6P	159271-83-7P	159271-84-8P
159271-85-9P	159271-86-0P	159271-87-1P	159271-88-2P
159271-89-3P	159271-90-6P	159271-91-7P	159271-92-8P
159271-93-9P	159271-94-0P	159271-95-1P	159271-96-2P
159271-97-3P	159271-98-4P	159271-99-5P	159272-00-1P
159272-01-2P	159272-02-3P	159272-03-4P	159272-04-5P
159272-05-6P	159272-06-7P	159272-07-8P	159272-08-9P
159272-09-0P	159272-10-3P	159272-11-4P	159272-12-5P
159272-13-6P	159272-14-7P	159272-15-8P	159272-16-9P
159272-17-0P	159272-18-1P	159272-19-2P	159272-20-5P

ROLE: BAC (Biological activity or effector, except

adverse);

SPN (Synthetic preparation); THU (Therapeutic use); BIOL  
(Biological study); PREP (Preparation); USES (Uses)  
(prepn. of phosphonic acid derivs. useful for medically  
treating hyperlipemia)

INDEX TERM:

159272-21-6P	159272-22-7P	159272-23-8P	159272-24-9P
159272-25-0P	159272-26-1P	159272-27-2P	159272-28-3P
159272-29-4P	159272-30-7P	159272-31-8P	159272-32-9P
159272-33-0P	159272-34-1P	159272-35-2P	159272-36-3P
159272-37-4P	159272-38-5P	159272-39-6P	159272-40-9P
159272-41-0P	159272-42-1P	159272-43-2P	159272-44-3P
159272-45-4P	159272-46-5P	159272-47-6P	159272-48-7P
159272-49-8P	159272-50-1P	159272-51-2P	159272-52-3P
159272-53-4P	159272-54-5P	159272-55-6P	159272-56-7P
159272-57-8P	159272-58-9P	159272-59-0P	159272-60-3P
159272-61-4P	159272-62-5P	159272-63-6P	159272-64-7P
159272-65-8P	159272-66-9P	159272-67-0P	159272-68-1P
159272-69-2P	159272-70-5P	159272-71-6P	159272-72-7P
159272-73-8P	159272-74-9P	159272-75-0P	159272-76-1P
159272-77-2P	159272-78-3P	159272-79-4P	159272-80-7P
159272-81-8P	159272-82-9P	159272-83-0P	159272-84-1P
159272-85-2P	159272-86-3P	159272-87-4P	159272-88-5P
159272-89-6P	159272-90-9P	159272-91-0P	159272-92-1P
159272-93-2P	159272-94-3P	159272-95-4P	159272-96-5P



159272-97-6P	159272-98-7P	159272-99-8P	159273-00-4P
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159273-85-5P	159273-86-6P	159273-87-7P	159273-88-8P
159273-89-9P	159273-90-2P	159273-91-3P	159273-92-4P
159273-93-5P	159273-94-6P	159273-95-7P	159273-96-8P
159273-97-9P	159273-98-0P	159273-99-1P	159274-00-7P
159274-01-8P	159274-02-9P	159274-03-0P	159274-04-1P
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159274-45-0P	159274-46-1P	159274-47-2P	159274-48-3P
159274-49-4P	159274-50-7P	159274-51-8P	159274-52-9P
159274-53-0P	159274-54-1P	159274-55-2P	

ROLE: BAC (Biological activity or effector, except

adverse);

SPN (Synthetic preparation); THU (Therapeutic use); BIOL  
(Biological study); PREP (Preparation); USES (Uses)  
(prepn. of phosphonic acid derivs. useful for medically  
treating hyperlipemia)

INDEX TERM:

159274-56-3P	159274-57-4P	159274-58-5P	159274-59-6P
159274-60-9P	159274-61-0P	159274-62-1P	159274-63-2P
159274-64-3P	159274-65-4P	159274-66-5P	159274-67-6P
159274-68-7P	159274-69-8P	159274-70-1P	159274-71-2P
159274-72-3P	159274-73-4P	159274-74-5P	159274-75-6P
159274-76-7P	159274-77-8P	159274-78-9P	159274-80-3P
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159274-89-2P	159274-90-5P	159274-91-6P	159274-92-7P

159274-93-8P 159274-94-9P 159274-95-0P 159274-96-1P  
 159274-97-2P 159274-98-3P 159274-99-4P 159275-00-0P  
 159275-01-1P 159275-02-2P 159275-03-3P 159275-04-4P  
 159275-05-5P 159275-06-6P 159275-08-8P 159275-09-9P  
 159275-10-2P 159275-11-3P 159275-12-4P 159275-13-5P  
 ROLE: BAC (Biological activity or effector, except

adverse);

SPN (Synthetic preparation); THU (Therapeutic use); BIOL  
 (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of phosphonic acid derivs. useful for medically  
 treating hyperlipemia)

INDEX TERM:  
 98-59-9,

68-12-2, reactions 91-57-6, 2-Methylnaphthalene

p-Toluenesulfonyl chloride 98-88-4, Benzoyl chloride  
 103-67-3, N-Methylbenzylamine 108-39-4, reactions  
 109-70-6, 1-Bromo-3-chloropropane 122-51-0, Ethyl  
 orthoformate 124-63-0, Methanesulfonyl chloride  
 141-97-9, Ethyl acetoacetate 501-53-1 762-04-9, Diethyl  
 phosphite 814-49-3, Diethyl chlorophosphate 821-11-4  
 867-13-0, Triethyl phosphonoacetate 1660-94-2, Tetraethyl  
 methylenediphosphonate 1885-14-9, Phenyl chloroformate  
 2045-79-6 2620-50-0, Piperonylamine 2857-97-8,  
 Trimethylsilyl bromide 3682-19-7 3796-70-1 6117-80-2  
 6457-49-4, 4-Piperidinemethanol 7087-68-5,  
 N,N-Diisopropylethylamine 7693-46-1 10416-59-8  
 25519-78-2 33821-94-2 40681-88-7 53064-79-2,  
 Iodomethyl pivalate 58479-61-1 63343-64-6 76362-12-4  
 79026-11-2 108298-18-6 111773-01-4 119402-67-4  
 141816-04-8 150250-34-3 150250-35-4 159275-46-4  
 159275-47-5 159275-48-6 159275-49-7 159275-50-0

ROLE: RCT (Reactant)

(prepn. of phosphonic acid derivs. useful for medically  
 treating hyperlipemia)

INDEX TERM:

614-32-4P 939-26-4P 3161-52-2P 65109-84-4P  
 68427-26-9P 122860-33-7P 123802-05-1P 152126-99-3P  
 159275-14-6P 159275-15-7P 159275-16-8P 159275-17-9P  
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 159275-42-0P 159275-43-1P 159275-44-2P 159275-45-3P  
 159275-52-2P 159275-53-3P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation)

(prepn. of phosphonic acid derivs. useful for medically  
 treating hyperlipemia)

INDEX TERM:

159275-07-7P 159275-51-1P

ROLE: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of phosphonic acid derivs. useful for medically  
 treating hyperlipemia)

IT 159270-75-4P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic  
 preparation); THU (Therapeutic use); BIOL (Biological study); PREP

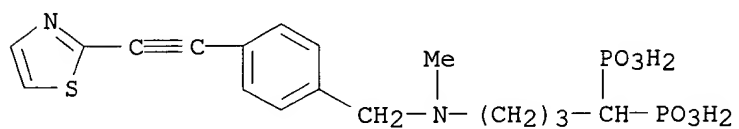
(Preparation); USES (Uses)

(prepn. of phosphonic acid derivs. useful for medically treating hyperlipemia)

RN 159270-75-4 CAPLUS

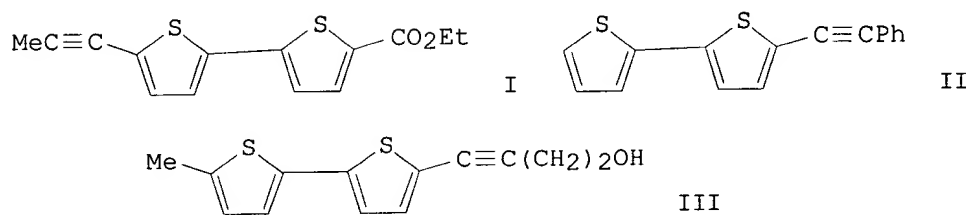
CN Phosphonic acid,

[4-[methyl[[4-(2-thiazolylethynyl)phenyl]methyl]amino]butylidene]bis-, tetrasodium salt (9CI) (CA INDEX NAME)



● 4 Na

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2001 ACS  
 ACCESSION NUMBER: 1989:185340 CAPLUS  
 DOCUMENT NUMBER: 110:185340  
 TITLE: **Antiviral properties of acetylenes and thiophenes**  
 AUTHOR(S): Hudson, J. B.; Towers, G. H. N.  
 CORPORATE SOURCE: Dep. Bot., Univ. British Columbia, Vancouver, BC, Can.  
 SOURCE: Bioact. Mol. (1988), 7 (Chem. Biol. Nat.-Occurring Acetylenes Relat. Compd.), 315-38  
 CODEN: BMOLEY; ISSN: 0921-0687  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 CLASSIFICATION: 1-3 (Pharmacology)  
 GRAPHIC IMAGE:



# ABSTRACT:

A series of 31 synthetic **thiophenes** was tested for antiviral activity in vitro using Sinbis virus or murine cytomegalovirus infection of murine 3T3-L1 cells and std. UV-A exposure as the test system. None of the compds. were active in the dark. I was the most potent inhibitor of Sindbis virus, and II and III were the most active against murine cytomegalovirus. In general, there was a fairly good agreement between the results for the 2 viruses. Structure-activity relationships are discussed. The antiviral activities of 5 addnl. compds. (thiarubrine A, thiophene A, .alpha.-terthienyl, phenylheptatriyne, and ACBP-thiophene) are reviewed.

SUPPL. TERM: antiviral activity thiophene acetylene structure  
 INDEX TERM: Virucides and Virustats  
                   (acetylenes and thiophenes,  
                   light-dependent)  
 INDEX TERM: Photodynamic action  
                   (virucidal, of acetylene and **thiophenes**,  
                   structure in relation to)  
 INDEX TERM: Molecular structure-biological activity relationship  
                   (virucidal, of **acetylenes** and  
                   **thiophenes**, light-dependent)  
 INDEX TERM: 886-66-8 1081-34-1, .alpha.-Terthienyl 1137-87-7  
 1152-72-3 1204-82-6 1665-29-8 1665-35-6 2134-99-8,  
 Thiophene A 3172-56-3, 3,3'-Bithiophene 4300-27-0,  
 Phenylheptatriyne 4805-17-8 4805-21-4  
 16278-95-8 16900-51-9 32155-99-0 58930-55-5  
 63543-09-9 88089-34-3 90267-18-8 90920-85-7

93297-79-1 93297-81-5 94742-65-1 94742-70-8  
 100074-13-3 105124-97-8, 3,2':4',3''-Terthiophene  
 105124-98-9, 3,3':4',3''-Terthiophene 105124-99-0  
 105125-00-6 105125-03-9 105125-04-0 106032-17-1,  
 3,2':3',3''-Terthiophene 117205-69-3 120381-53-5  
 120381-54-6 120381-55-7

ROLE: BAC (Biological activity or effector, except

adverse);

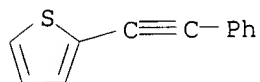
THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (virucidal activity of, light-dependent, structure in  
 relation to)

IT 4805-17-8 4805-21-4 90267-18-8

RL: BAC (Biological activity or effector, except adverse); THU  
 (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (virucidal activity of, light-dependent, structure in relation to)

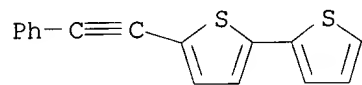
RN 4805-17-8 CAPLUS

CN Thiophene, 2-(phenylethynyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)



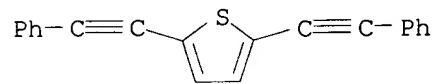
RN 4805-21-4 CAPLUS

CN 2,2'-Bithiophene, 5-(phenylethynyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)

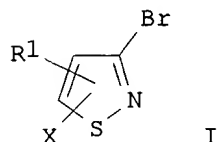


RN 90267-18-8 CAPLUS

CN Thiophene, 2,5-bis(phenylethynyl)- (9CI) (CA INDEX NAME)



L15 ANSWER 20 OF 46 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1998:272663 CAPLUS  
 DOCUMENT NUMBER: 128:321593  
 TITLE: Alkynylisothiazoles  
 AUTHOR(S): Zlotin, S. G.; Kislitsin, P. G.; Luk'yanov, O. A.  
 CORPORATE SOURCE: N. D. Zelinsky Institute of Organic Chemistry,  
 Russian Academy of Sciences, Moscow, 117913, Russia  
 SOURCE: Russ. Chem. Bull. (1998), 47(3), 519-523  
 CODEN: RCBUEY; ISSN: 1066-5285  
 PUBLISHER: Consultants Bureau  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 CLASSIFICATION: 28-7 (Heterocyclic Compounds (More Than One Hetero  
 Atom))  
 GRAPHIC IMAGE:



ABSTRACT:

A new synthesis of mono- and dialkynylisothiazoles I ( $R_1 = 4\text{-Br}, 4\text{-iodo}, 5\text{-H}, 5\text{-Ph}$ ;  $\text{C.tplbond.C}$ ,  $X = \text{C.tplbond.CR}_2$ ,  $R_2 = \text{Ph}, n\text{-hexyl}, \text{CH}_2\text{OH}, \text{CH}_2\text{OMe}$ ) by cross-coupling of bromine- and iodine-contg. isothiazoles with terminal acetylene moieties in the  $\text{PdCl}_2(\text{PPh}_3)_2\text{-CuI-NEt}_3$  catalytic system has been developed.

SUPPL. TERM: coupling haloisothiazole acetylene palladium;  
 alkynylisothiazole prepn palladium catalyst; isothiazole  
 alkynyl prepn palladium catalyst  
 INDEX TERM: 107-19-7, Propargyl alcohol 536-74-3, Phenylacetylene  
 627-41-8 629-05-0, 1-Octyne 71091-87-7 202287-55-6  
 202287-56-7  
 ROLE: RCT (Reactant)  
 (palladium-catalyzed cross-coupling of haloisothiazoles  
 with acetylenes)  
 INDEX TERM: 202287-54-5P 207000-19-9P **207000-21-3P**  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (palladium-catalyzed cross-coupling of haloisothiazoles  
 with acetylenes)  
 INDEX TERM: 886-66-8P **207000-17-7P** 207000-18-8P  
 207000-20-2P 207000-22-4P **207000-23-5P**  
**207000-24-6P** 207000-25-7P  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (palladium-catalyzed cross-coupling of haloisothiazoles

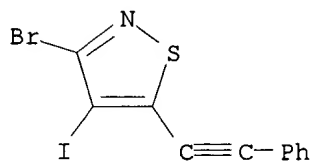
with acetylenes)

IT 207000-21-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(palladium-catalyzed cross-coupling of haloisothiazoles with  
acetylenes)

RN 207000-21-3 CAPLUS

CN Isothiazole, 3-bromo-4-iodo-5-(phenylethynyl)- (9CI) (CA INDEX NAME)

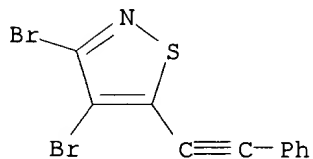


IT 207000-17-7P 207000-23-5P 207000-24-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(palladium-catalyzed cross-coupling of haloisothiazoles with  
acetylenes)

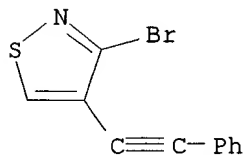
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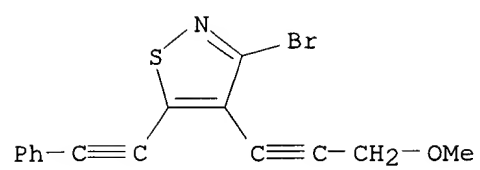
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CN Isothiazole, 3-bromo-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



RN 207000-24-6 CAPLUS

CN Isothiazole, 3-bromo-4-(3-methoxy-1-propynyl)-5-(phenylethynyl)- (9CI)  
(CA INDEX NAME)





L15 ANSWER 15 OF 46 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:733991 CAPLUS

DOCUMENT NUMBER: 132:22906

TITLE: 2-Substituted 5-acetyl-4-thiazolyl triflates as  
useful

building blocks for the preparation of functionalized  
thiazoles

AUTHOR(S): Arcadi, Antonio; Attanasi, Orazio A.; Guidi, Barbara;  
Rossi, Elisabetta; Santeusano, Stefania

CORPORATE SOURCE: Dipartimento Chimica, Ingegneria Chimica Materiali,  
Univ. L'Aquila, L'Aquila, I-67100, Italy

SOURCE: Eur. J. Org. Chem. (1999), (11), 3117-3126

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 28-7 (Heterocyclic Compounds (More Than One Hetero  
Atom))

OTHER SOURCE(S): CASREACT 132:22906

ABSTRACT:

Readily available 2-substituted 5-acetyl-4-thiazolyl triflates (I) are useful building blocks for the prepn. of functionalized thiazoles by Pd-catalyzed cross-coupling reactions with organometallic reagents and alkoxycarbonylation and deoxygenation reactions. The combination of Pd-catalyzed coupling of I together with 1-alkynes/6-endo-dig annulation reactions in the presence of NH<sub>3</sub> leads to functionalized pyrido[3,4-c]thiazoles in satisfactory yields. The utilization of uncatalyzed displacement reactions of the triflate group represents a very simple method for the synthesis of 4-N-, 4-O-, and 4-S-substituted thiazoles.

SUPPL. TERM: thiazole prepn; thiazolyl triflate palladium catalyzed  
cross

coupling

INDEX TERM: 77-75-8, 3-Methyl-1-pentyn-3-ol 78-27-3,  
1-Ethynylcyclohexanol 98-80-6, Phenylboronic acid  
100-63-0, Phenylhydrazine 110-89-4, Piperidine, reactions  
110-91-8, Morpholine, reactions 536-74-3, Phenylacetylene  
629-05-0, 1-Octyne 6258-60-2,

4-Methoxybenzenemethanethiol

7486-35-3, Tributylvinylstannane 10160-87-9,  
3,3-Diethoxy-1-propyne 54663-78-4, 2-  
(Tributylstannyl)thiophene 87199-16-4,  
3-Formylphenylboronic acid 207397-53-3 207397-54-4  
207397-55-5 207397-56-6 207397-57-7 207397-58-8  
207397-59-9

ROLE: RCT (Reactant)

(prepn. of thiazoles via acetylthiazolyl triflates)

INDEX TERM: 220449-50-3P 220449-51-4P 220449-52-5P 220449-53-6P

220449-54-7P 220449-55-8P 220449-56-9P

**220449-57-0P** 220449-59-2P 220449-60-5P

**220449-61-6P 220449-62-7P**

**220449-63-8P 220449-64-9P** 220449-65-0P

**220449-66-1P 220449-67-2P**

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation)  
 (prepn. of thiazoles via acetylthiazolyl triflates)

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 252013-21-1P 252013-22-2P

ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of thiazoles via acetylthiazolyl triflates)

REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD.

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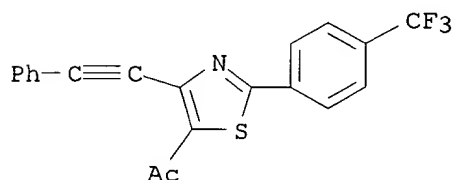
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 220449-67-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of thiazoles via acetylthiazolyl triflates)

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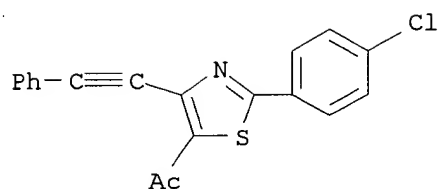
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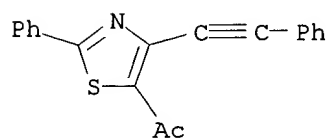
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 (CA

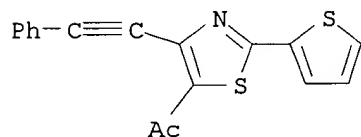
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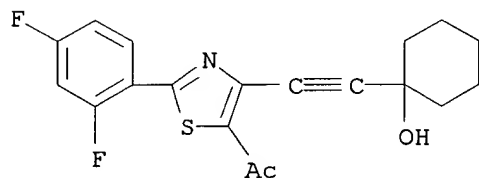
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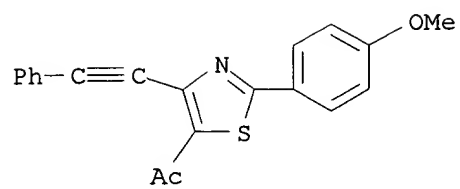
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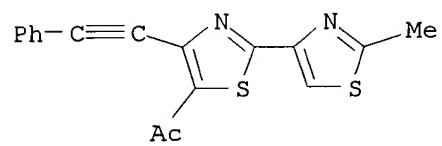
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RN 220449-67-2 CAPLUS

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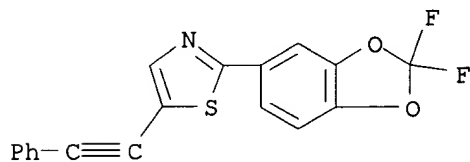
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INDEX NAME)



L34 ANSWER 18 OF 20 USPATFULL  
 AN 88:77501 USPATFULL  
 TI Photoactivated miticidal and insecticidal ethynylthiazoles  
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 Roush, David M., Princeton, NJ, United States  
 Phillips, Richard B., Diamond Bar, CA, United States  
 PA FMC Corporation, Philadelphia, PA, United States (U.S. corporation)  
 PI US 4788207 19881129  
 AI US 1988-161867 19880229 (7)  
 DT Utility  
 FS Granted  
 LN.CNT 525  
 INCL INCLM: 514/365.000  
 INCLS: 548/202.000; 548/203.000  
 NCL NCLM: 514/365.000  
 NCLS: 548/202.000; 548/203.000  
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 ICS: C07D277-22; A01N043-78  
 EXF 548/202; 548/203; 514/365  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.

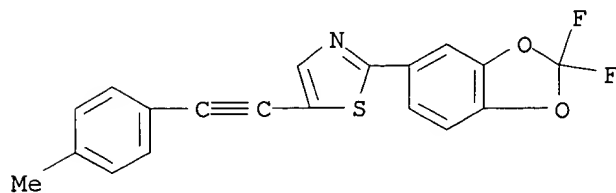
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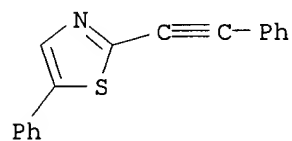


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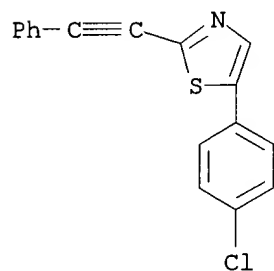
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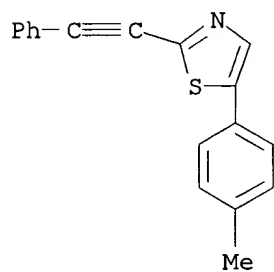
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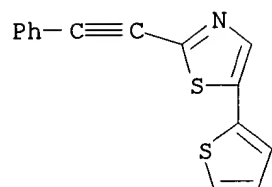


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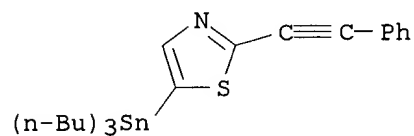
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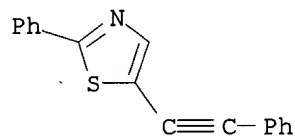
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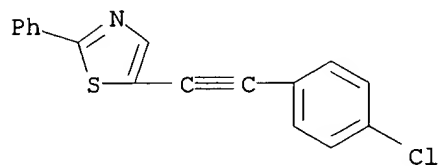
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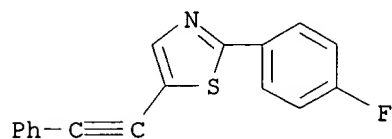
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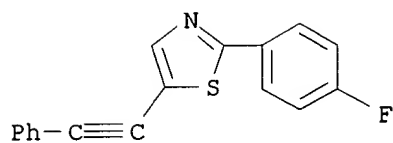


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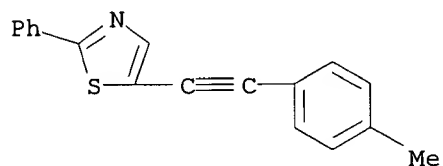
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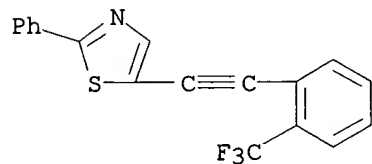




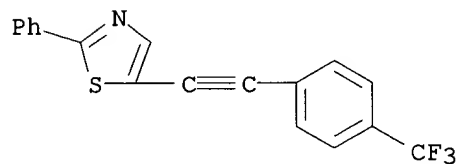
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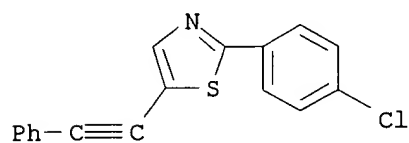
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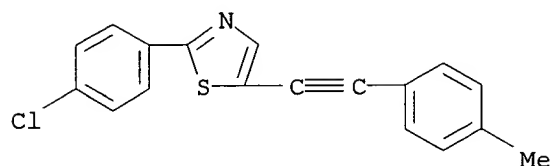
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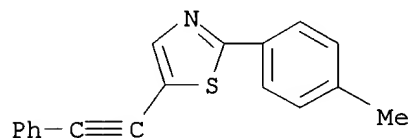
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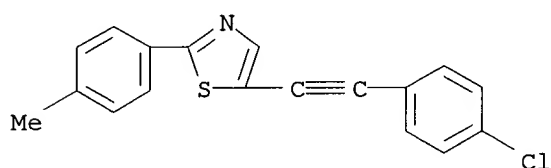
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INDEX NAME)



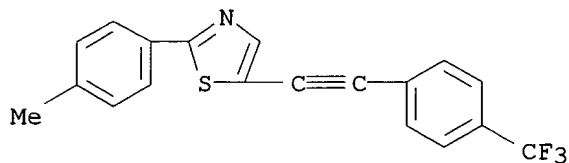
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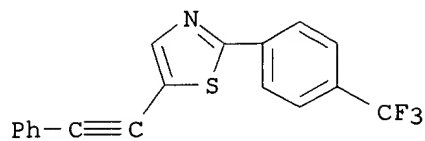


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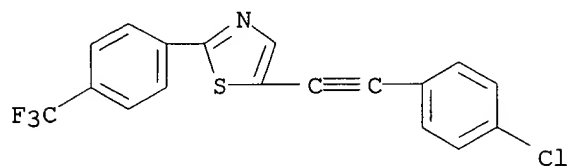
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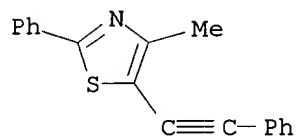
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(CA INDEX NAME)



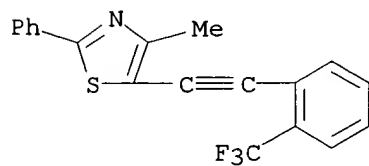
RN 119514-42-0 USPATFULL

CN Thiazole, 4-methyl-2-phenyl-5-(phenylethynyl)- (9CI) (CA INDEX NAME)



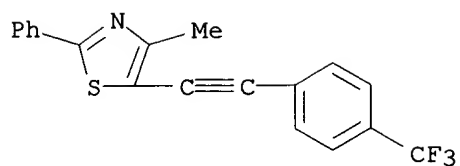
RN 119514-43-1 USPATFULL

CN Thiazole, 4-methyl-2-phenyl-5-[[2-(trifluoromethyl)phenyl]ethynyl]- (9CI)  
(CA INDEX NAME)

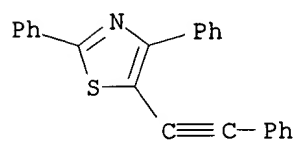


RN 119514-44-2 USPATFULL

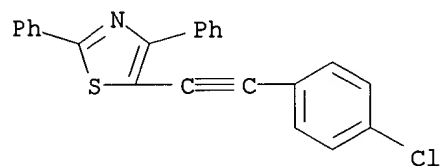
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(CA INDEX NAME)



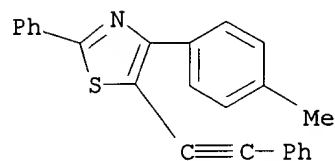
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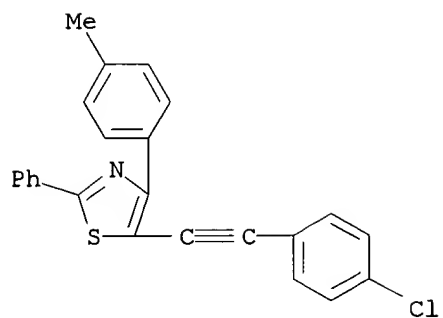
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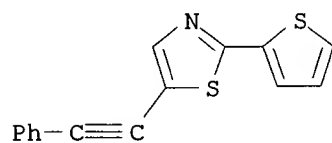
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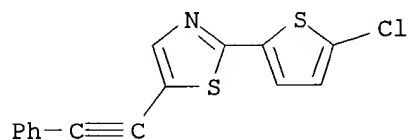
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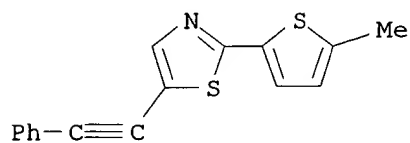
RN 119514-49-7 USPATFULL  
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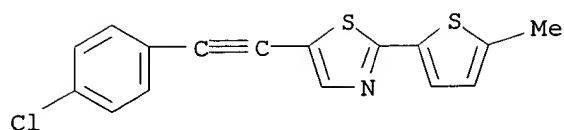
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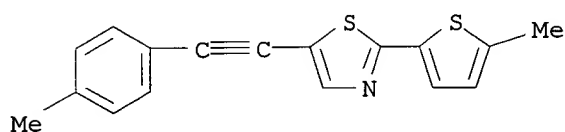
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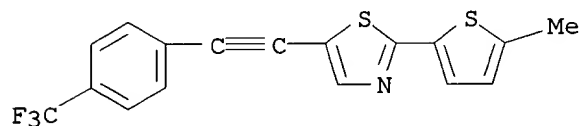
RN 119514-52-2 USPATFULL  
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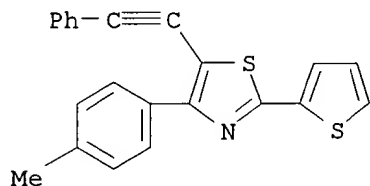
RN 119514-53-3 USPATFULL  
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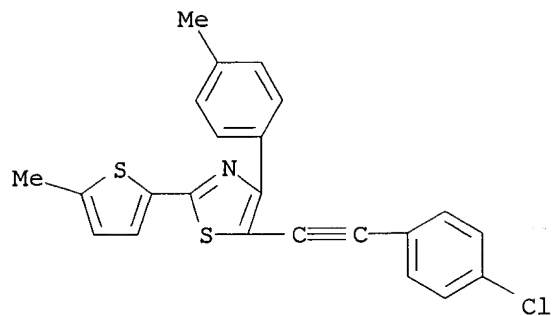
RN 119514-54-4 USPATFULL  
 CN Thiazole, 2-(5-methyl-2-thienyl)-5-[[4-(trifluoromethyl)phenyl]ethynyl]- (9CI) (CA INDEX NAME)



RN 119514-55-5 USPATFULL  
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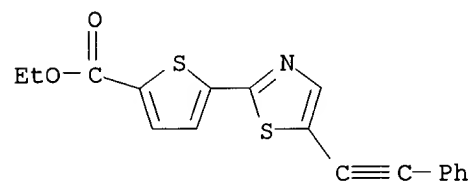


RN 119514-56-6 USPATFULL  
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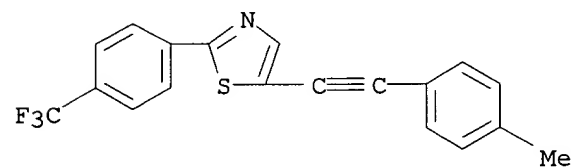
RN 119514-57-7 USPATFULL

CN 2-Thiophenecarboxylic acid, 5-[5-(phenylethynyl)-2-thiazolyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 119539-82-1 USPATFULL

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(CA INDEX NAME)

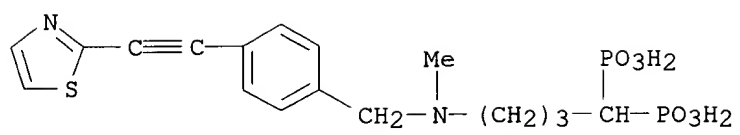


L31 ANSWER 10 OF 10 USPATFULL  
 AN 1998:17462 USPATFULL  
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 IN Yoshida, Ichirou, Ibaraki, Japan  
 Ikuta, Hironori, Ibaraki, Japan  
 Fukuda, Yoshio, Ibaraki, Japan  
 Eguchi, Yoshihito, Ibaraki, Japan  
 Kaino, Makoto, Ibaraki, Japan  
 Tagami, Katsuya, Arlington, MA, United States  
 Kobayashi, Naoki, Ibaraki, Japan  
 Hayashi, Kenji, Ibaraki, Japan  
 Hiyoshi, Hironobu, Ibaraki, Japan  
 Ohtsuka, Issei, Ibaraki, Japan  
 Nakagawa, Makoto, Ibaraki, Japan  
 Abe, Shinya, Ibaraki, Japan  
 Souda, Shigeru, Ibaraki, Japan  
 PA Eisai Co., Ltd., Tokyo, Japan (non-U.S. corporation)  
 PI US 5719303 19980217  
 WO 9420508 19940915  
 AI US 1995-530311 19950906 (8)  
 WO 1994-JP354 19940304  
 19950906 PCT 371 date  
 19950906 PCT 102(e) date  
 PRAI JP 1993-46389 19930308  
 DT Utility  
 FS Granted  
 LN.CNT 7489  
 INCL INCLM: 558/158.000  
 INCLS: 562/013.000  
 NCL NCLM: 558/158.000  
 NCLS: 562/013.000  
 IC [6]  
 ICM: C07F009-40  
 ICS: C07F009-38  
 EXF 562/13; 558/158  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.

=> d 10 hitstr

L31 ANSWER 10 OF 10 USPATFULL  
 IT **159270-75-4P**  
 (prepn. of phosphonic acid derivs. useful for medically treating  
 hyperlipemia)  
 RN 159270-75-4 USPATFULL  
 CN Phosphonic acid,  
 [4-[methyl[[4-(2-thiazolyethynyl)phenyl]methyl]amino]but  
 ylidene]bis-, tetrasodium salt (9CI) (CA INDEX NAME)



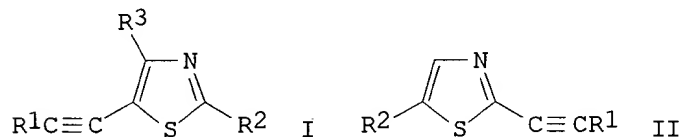


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L15 ANSWER 42 OF 46 CAPLUS COPYRIGHT 2002 ACS DUPLICATE 5  
 ACCESSION NUMBER: 1989:135230 CAPLUS  
 DOCUMENT NUMBER: 110:135230  
 TITLE: Preparation of ethynylthiazoles as photodynamic insecticides and acaricides  
 INVENTOR(S): Lutomski, Kathryn A.; Roush, David M.; Phillips, Richard B.  
 PATENT ASSIGNEE(S): FMC Corp., USA  
 SOURCE: U.S., 7 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 INT. PATENT CLASSIF.:  
 MAIN: C07D417-06  
 SECONDARY: C07D277-22; A01N043-78  
 US PATENT CLASSIF.: 514365000  
 CLASSIFICATION: 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 5  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4788207	A	19881129	US 1988-161867	19880229

OTHER SOURCE(S): CASREACT 110:135230; MARPAT 110:135230  
 GRAPHIC IMAGE:



# ABSTRACT:

Thirty-nine title 5-ethynylthiazoles I [R1 = C1-6 alkyl, methylthienyl, Me3Si, (un)substituted Ph; R2 = (un)substituted Ph, thienyl; R3 = H, C1-4 alkyl, Ph, MeC6H4] and nine isomeric 2-ethynylthiazoles II [R1 = Ph, alkylthienyl; R2 = (methyl)thienyl, trialkylstannyl, (un)substituted Ph] were prepd. as photoactivated miticides and insecticides. 4-ClC6H4CONH2 was sulfurated by refluxing 2 h in PhMe with Lawesson's reagent and cyclocondensed with BrCH2CH(OMe)2 by refluxing .apprx.3 days in EtOH in the presence of concd. HCl to give 2-(4-chlorophenyl)thiazole. The latter was metalated with BuLi at -78.degree.C in Et2O and treated with 1,2-diiodoethane to give the corresponding 5-iodothiazole which was refluxed 2 days with PhC.tplbond.CH in MeCN in the presence of Et3N, [Ph3P] PdCl2, and CuI to give I (R1 = Ph, R2 = 4-ClC6H4; R3 = H) (III). At 50 ppm III gave 100% kill of Tetranychus urticae and 20% kill of Trichoplusia ni after 48 h UV light exposure.

SUPPL. TERM: ethynylthiazole prepn miticide insecticide photosensitized  
 INDEX TERM: Acaricides

Insecticides  
(ethynylthiazoles)

INDEX TERM: 624-31-7P 2521-24-6P 3034-53-5P 27149-26-4P  
42140-95-4P 72505-21-6P 119514-22-6P 119514-23-7P  
119514-24-8P 119514-25-9P 119514-26-0P 119514-28-2P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation)  
(prepn. and reaction of, in prepn. of insecticides and  
acaricides)

INDEX TERM: 119514-10-2P **119514-11-3P 119514-12-4P**  
119514-13-5P 119514-14-6P 119514-15-7P 119514-16-8P  
119514-17-9P 119514-18-0P 119514-19-1P 119514-20-4P  
119514-21-5P 119514-28-2P **119514-29-3P**  
**119514-30-6P 119514-31-7P**  
**119514-32-8P 119514-33-9P**  
**119514-34-0P 119514-35-1P**  
**119514-36-2P 119514-37-3P**  
**119514-38-4P 119514-39-5P**  
**119514-40-8P 119514-41-9P**  
**119514-42-0P 119514-43-1P**  
**119514-44-2P 119514-45-3P**  
**119514-46-4P 119514-47-5P**  
**119514-48-6P 119514-49-7P**  
**119514-50-0P 119514-51-1P**  
**119514-52-2P 119514-53-3P**  
**119514-54-4P 119514-55-5P**  
**119514-56-6P 119514-57-7P** 119514-58-8P  
119514-59-9P 119514-60-2P **119514-61-3P**  
**119539-82-1P**  
ROLE: AGR (Agricultural use); BAC (Biological activity or  
effector, except adverse); SPN (Synthetic preparation);

BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of, as insecticide and acaricide)

INDEX TERM: 455-18-5, 4-(Trifluoromethyl)benzonitrile 536-74-3,  
Phenylacetylene 541-41-3, Ethyl chloroformate 619-56-7,  
4-Chlorobenzamide 624-73-7, 1,2-Diiodoethane 1066-54-2,  
(Trimethylsilyl)acetylene 5813-89-8, 2-  
Thiophenecarboxamide 7252-83-7, Bromoacetaldehyde

dimethyl acetal 16494-36-3, 2-Iodo-5-methylthiophene 17157-48-1,  
Bromoacetaldehyde 119514-27-1, 2-[(5-Methyl-2-  
thienyl)ethynyl]thiazole  
ROLE: RCT (Reactant)  
(reaction of, in prepn. of insecticides and acaricides)

IT **119514-11-3P 119514-12-4P 119514-29-3P**  
**119514-30-6P 119514-31-7P 119514-32-8P**  
**119514-33-9P 119514-34-0P 119514-35-1P**  
**119514-36-2P 119514-37-3P 119514-38-4P**  
**119514-39-5P 119514-40-8P 119514-41-9P**  
**119514-42-0P 119514-43-1P 119514-44-2P**  
**119514-45-3P 119514-46-4P 119514-47-5P**  
**119514-48-6P 119514-49-7P 119514-50-0P**  
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**119514-54-4P 119514-55-5P 119514-56-6P**

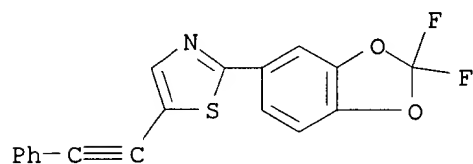
**119514-57-7P 119514-61-3P 119539-82-1P**

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as insecticide and acaricide)

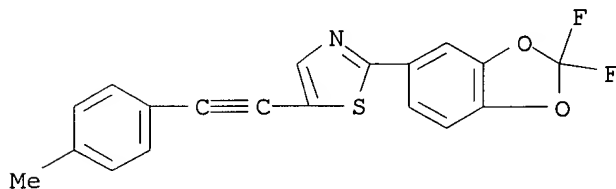
RN 119514-11-3 CAPLUS

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(CA INDEX NAME)



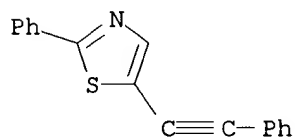
RN 119514-12-4 CAPLUS

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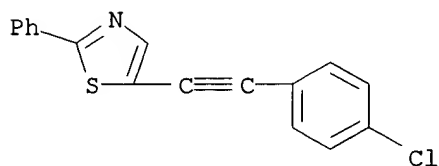
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CN Thiazole, 2-phenyl-5-(phenylethynyl)- (9CI) (CA INDEX NAME)

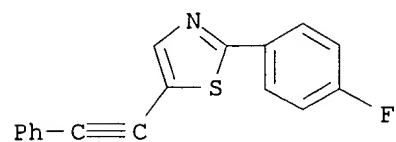


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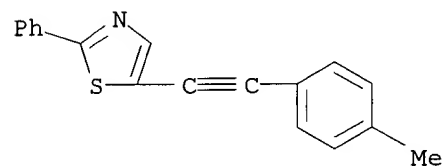
CN Thiazole, 5-[(4-chlorophenyl)ethynyl]-2-phenyl- (9CI) (CA INDEX NAME)



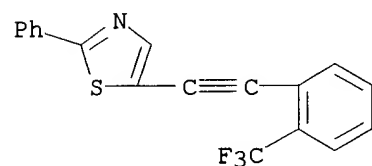
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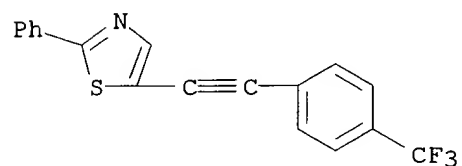
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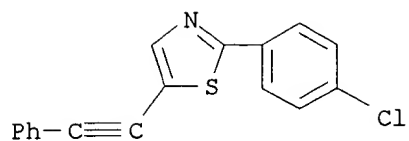
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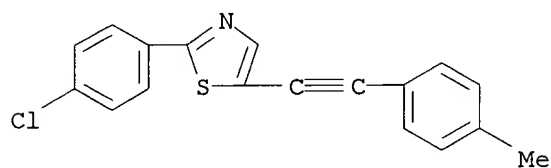
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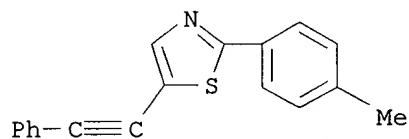
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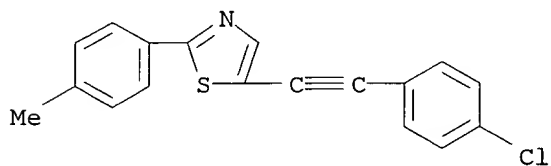
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 INDEX  
 NAME)



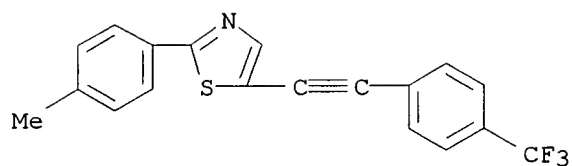
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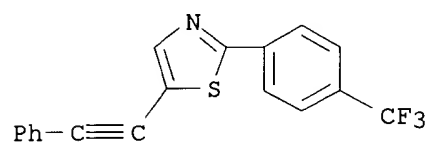
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 INDEX  
 NAME)



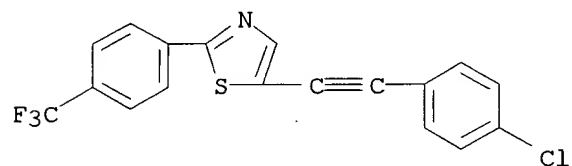
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 (9CI)  
 (CA INDEX NAME)



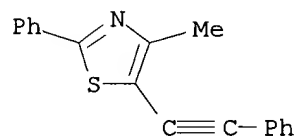
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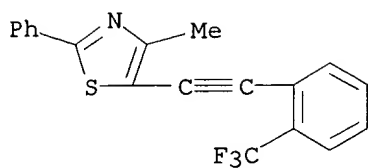
RN 119514-41-9 CAPLUS  
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 (CA INDEX NAME)



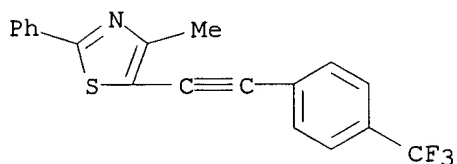
RN 119514-42-0 CAPLUS  
 CN Thiazole, 4-methyl-2-phenyl-5-(phenylethynyl)- (9CI) (CA INDEX NAME)



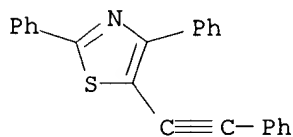
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 (CA INDEX NAME)



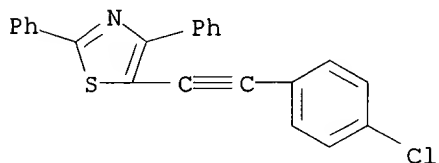
RN 119514-44-2 CAPLUS  
 CN Thiazole, 4-methyl-2-phenyl-5-[[4-(trifluoromethyl)phenyl]ethynyl]- (9CI)  
 (CA INDEX NAME)



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 CN Thiazole, 2,4-diphenyl-5-(phenylethynyl)- (9CI) (CA INDEX NAME)

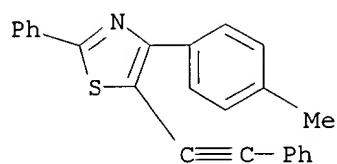


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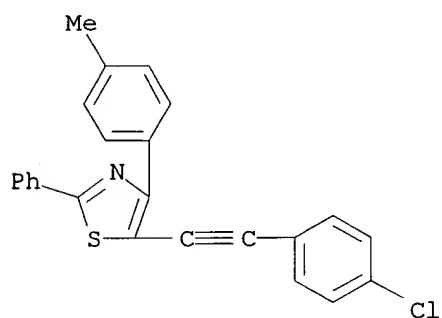


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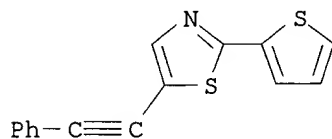




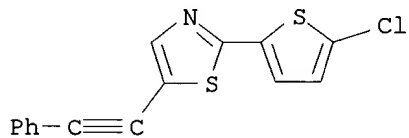
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 CN Thiazole, 5-[(4-chlorophenyl)ethynyl]-4-(4-methylphenyl)-2-phenyl- (9CI)  
 (CA INDEX NAME)



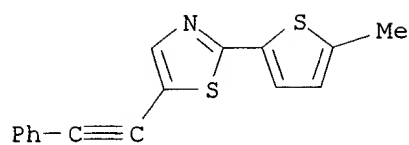
RN 119514-49-7 CAPLUS  
 CN Thiazole, 5-(phenylethynyl)-2-(2-thienyl)- (9CI) (CA INDEX NAME)



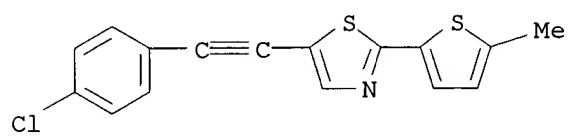
RN 119514-50-0 CAPLUS  
 CN Thiazole, 2-(5-chloro-2-thienyl)-5-(phenylethynyl)- (9CI) (CA INDEX NAME)



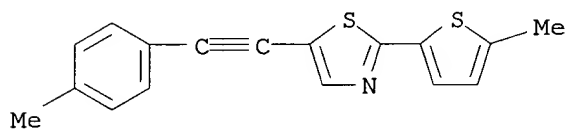
RN 119514-51-1 CAPLUS  
 CN Thiazole, 2-(5-methyl-2-thienyl)-5-(phenylethynyl)- (9CI) (CA INDEX NAME)



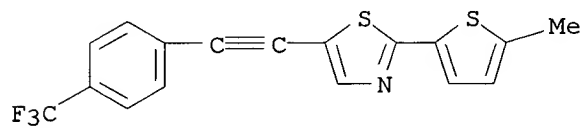
RN 119514-52-2 CAPLUS  
 CN Thiazole, 5-[(4-chlorophenyl)ethynyl]-2-(5-methyl-2-thienyl)- (9CI) (CA INDEX NAME)



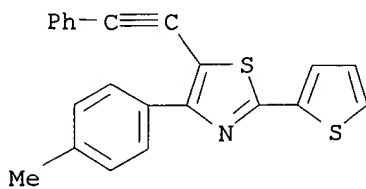
RN 119514-53-3 CAPLUS  
 CN Thiazole, 5-[(4-methylphenyl)ethynyl]-2-(5-methyl-2-thienyl)- (9CI) (CA INDEX NAME)

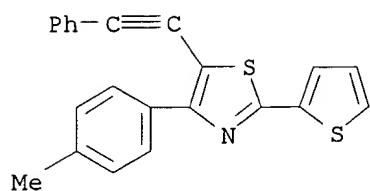


RN 119514-54-4 CAPLUS  
 CN Thiazole, 2-(5-methyl-2-thienyl)-5-[[4-(trifluoromethyl)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

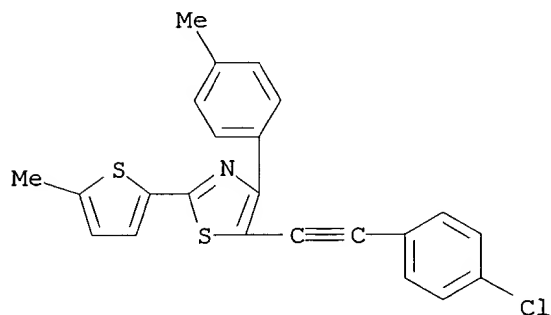


RN 119514-55-5 CAPLUS  
 CN Thiazole, 4-(4-methylphenyl)-5-(phenylethynyl)-2-(2-thienyl)- (9CI) (CA INDEX NAME)

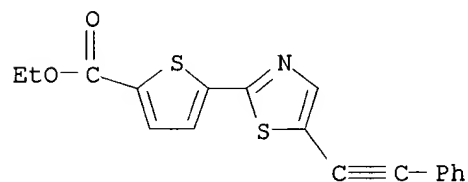




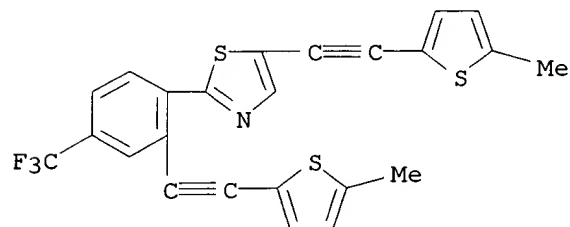
RN 119514-56-6 CAPLUS  
 CN Thiazole, 5-[(4-chlorophenyl)ethynyl]-4-(4-methylphenyl)-2-(5-methyl-2-thienyl)- (9CI) (CA INDEX NAME)



RN 119514-57-7 CAPLUS  
 CN 2-Thiophenecarboxylic acid, 5-[5-(phenylethynyl)-2-thiazolyl]-, ethyl ester (9CI) (CA INDEX NAME)



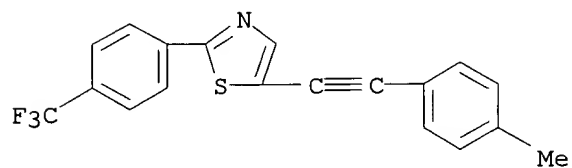
RN 119514-61-3 CAPLUS  
 CN Thiazole, 5-[(5-methyl-2-thienyl)ethynyl]-2-[2-[(5-methyl-2-thienyl)ethynyl]-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 119539-82-1 CAPLUS

CN Thiazole, 5-[(4-methylphenyl)ethynyl]-2-[4-(trifluoromethyl)phenyl]-  
(9CI)

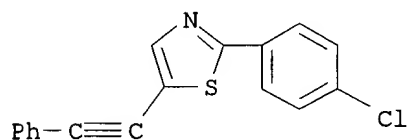
(CA INDEX NAME)



L34 ANSWER 17 OF 20 USPATFULL  
 AN 89:102251 USPATFULL  
 TI Photoactivated miticidal and insecticidal ethynyl-thiazoles  
 IN Lutomski, Kathryn A., Hightstown, NJ, United States  
 Roush, David M., Princeton, NJ, United States  
 Phillips, Richard B., Irvine, CA, United States  
 PA FMC Corporation, Philadelphia, PA, United States (U.S. corporation)  
 PI US 4889867 19891226  
 AI US 1988-271809 19881115 (7)  
 DT Utility  
 FS Granted  
 LN.CNT 470  
 INCL INCLM: 514/365.000  
 INCLS: 548/202.000; 548/203.000  
 NCL NCLM: 514/365.000  
 NCLS: 548/202.000; 548/203.000  
 IC [4]  
 ICM: A01N043-78  
 ICS: C07D417-06; C07D277-22  
 EXF 514/365; 548/202; 548/203  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.

=> d 134 17 hitstr

L34 ANSWER 17 OF 20 USPATFULL  
 IT **119514-35-1P**  
 (prepn. of, as insecticide and acaricide)  
 RN 119514-35-1 USPATFULL  
 CN Thiazole, 2-(4-chlorophenyl)-5-(phenylethynyl)- (9CI) (CA INDEX NAME)



d 134 15

L34 ANSWER 15 OF 20 USPATFULL

AN 95:13889 USPATFULL

TI Acetylene derivatives, their preparation and their use for controlling insects and acaridae

IN Rentzea, Costin, Heidelberg, Germany, Federal Republic of  
Kardorff, Uwe, Mannheim, Germany, Federal Republic of  
Kuenast, Christoph, Otterstadt, Germany, Federal Republic of  
Theobald, Hans, Limburgerhof, Germany, Federal Republic of

PA BASF Aktiengesellschaft, Ludwigshafen, Germany, Federal Republic of  
(non-U.S. corporation)

PI US 5389656 19950214

AI US 1992-911386 19920713 (7)

RLI Continuation of Ser. No. US 1991-737866, filed on 30 Jul 1991, now abandoned

PRAI DE 1990-4024281 19900731

DT Utility

FS Granted

LN.CNT 733

INCL INCLM: 514/365.000

INCLS: 514/438.000; 548/202.000; 548/203.000; 549/074.000; 549/078.000;  
549/080.000

NCL NCLM: 514/365.000

NCLS: 514/438.000; 548/202.000; 548/203.000; 549/074.000; 549/078.000;  
549/080.000

IC [6]

ICM: C07D277-22

ICS: C07D333-08; A01N043-78; A01N043-10

EXF 548/202; 548/203; 549/74; 549/78; 549/80; 514/365; 514/438

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

=> d 134 15 hitstr

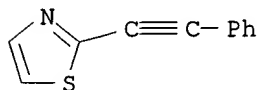
L34 ANSWER 15 OF 20 USPATFULL

IT **35070-01-0P**

(prepn. of, as acaricide and insecticide)

RN 35070-01-0 USPATFULL

CN Thiazole, 2-(phenylethynyl)- (9CI) (CA INDEX NAME)

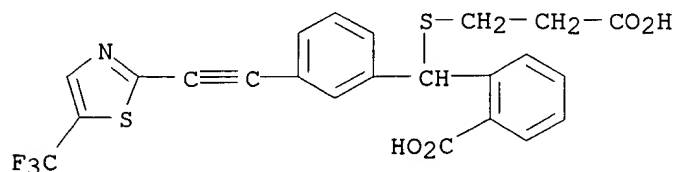


=>

L35 ANSWER 6 OF 6 USPATFULL  
 AN 90:78252 USPATFULL  
 TI Heterazole dialkanoic acids  
 IN Young, Robert N., Senneville, Canada  
 Atkinson, Joseph G., Montreal, Canada  
 PA Merck Frosst Canada, Inc., Kirkland, Canada (non-U.S. corporation)  
 PI US 4962117 19901009  
 AI US 1988-265972 19881102 (7)  
 RLI Continuation-in-part of Ser. No. US 1987-125622, filed on 25 Nov 1987,  
 now abandoned  
 DT Utility  
 FS Granted  
 LN.CNT 1044  
 INCL INCLM: 514/365.000  
 INCLS: 514/340.000; 514/341.000; 514/342.000; 514/369.000; 514/370.000;  
 514/371.000; 514/374.000; 514/376.000; 514/377.000; 514/182.000;  
 514/392.000; 514/398.000; 514/400.000; 546/275.000; 546/278.000;  
 546/280.000; 548/187.000; 548/194.000; 548/195.000; 548/200.000;  
 548/201.000; 548/204.000; 548/229.000; 548/233.000; 548/236.000;  
 548/252.000; 548/315.000; 548/337.000; 548/342.000  
 NCL NCLM: 514/365.000  
 NCLS: 514/340.000; 514/341.000; 514/342.000; 514/369.000; 514/370.000;  
 514/371.000; 514/374.000; 514/376.000; 514/377.000; 514/382.000;  
 514/392.000; 514/398.000; 514/400.000; 546/269.700; 546/270.700;  
 546/271.400; 546/272.700; 546/274.400; 546/274.700; 546/275.100;  
 548/187.000; 548/194.000; 548/195.000; 548/200.000; 548/201.000;  
 548/204.000; 548/229.000; 548/233.000  
 IC [5]  
 ICM: C07D277-30  
 ICS: C07D263-32; C07D233-26; A61K031-425  
 EXF 548/204; 548/236; 548/342; 548/252; 548/229; 548/195; 548/233; 548/337;  
 548/315; 548/187; 548/194; 548/200; 548/201; 546/278; 546/275; 546/280;  
 514/365; 514/369; 514/370; 514/371; 514/346; 514/341; 514/342; 514/374;  
 514/376; 514/377; 514/392; 514/398; 514/400  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.

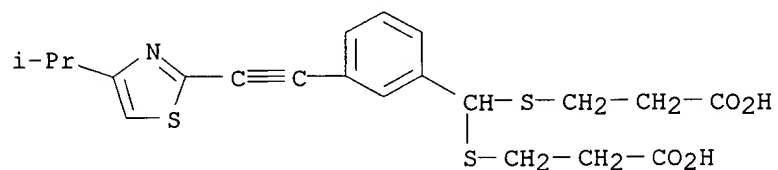
=> d 6 hitstr

L35 ANSWER 6 OF 6 USPATFULL  
 IT **126173-26-0P 126173-27-1P 126173-28-2P**  
 (prepn. of, as pharmaceutical)  
 RN 126173-26-0 USPATFULL  
 CN Benzoic acid, 2-[[[2-carboxyethyl)thio][3-[[5-(trifluoromethyl)-2-  
 thiazolyl]ethynyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



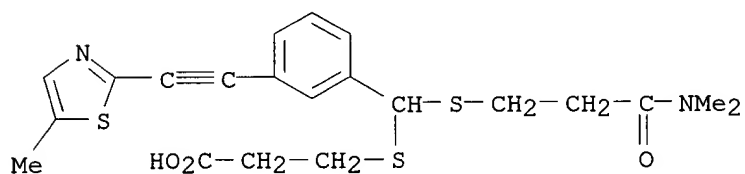
RN 126173-27-1 USPATFULL

CN Propanoic acid, 3,3'-[[[3-[[4-(1-methylethyl)-2-thiazolyl]ethynyl]phenyl]methylene]bis(thio)]bis- (9CI) (CA INDEX NAME)



RN 126173-28-2 USPATFULL

CN Propanoic acid, 3-[[[3-(dimethylamino)-3-oxopropyl]thio][3-[(5-methyl-2-thiazolyl)ethynyl]phenyl]methyl]thio]- (9CI) (CA INDEX NAME)





=&gt; d bib abs hitstr 164 1

**L64 ANSWER 1 OF 13 HCAPLUS** COPYRIGHT 2001 ACS

AN 1999:789712 HCAPLUS  
 DN 132:22765  
 TI Preparation of sulfonamides and TNF-.alpha. inhibitors  
 IN Watanabe, Fumihiko; Hamana, Hiroshi; Suzuki, Ryuji; Tsuzuki, Hiroshige  
 PA Shionogi Seiyaku K. K., Japan  
 SO Jpn. Kokai Tokkyo Koho, 37 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 11343279	A2	19991214	JP 1999-69892	19990316
PRAI	JP 1998-65040		19980316		

OS MARPAT 132:22765

AB R5R4R3SO2NR2CHR1(CH2)mX [R1 = (un)substituted lower alkyl, aryl, aralkyl, heteroaryl, etc.; R2 = H, lower alkyl, (CH2)tor27, aralkyl; t = 1-4; R27 = H, tetrahydropyranyl; R3 = (un)substituted arylene; heteroarylene, single bond; R4 (CH2)n, CH:CH, C.tplbond.C, CO, CONH, N:N, etc.; R5 = (un)substituted aryl, heteroaryl, alkyl, aralkyl, aralkyloxy, etc.; X = SR7, OR8, SCOR9, OCOR10, etc.; R7 = H, lower alkyl, aryl, heteroaryl, etc.; R8 = H, lower alkyl, lower alkylsulfonyl; R9, R10 = lower alkyl, aryl, heteroaryl, etc.], their optically active compds., their pharmaceutically acceptable salts, or their hydrates are prepd. (R)-3-(indol-3-yl)-1-mesyloxy-2-[N-[(4-phenoxyphenyl)sulfonyl]-N-methylamino]propane was reacted with potassium thioacetate in DMF at 50.degree. for 5 h to give 69% (R)-3-(indol-3-yl)-1-acetylthio-2-[N-[(4-phenoxyphenyl)sulfonyl]-N-methylamino]propane showing good inhibitory activity against TNF-.alpha. prodn.

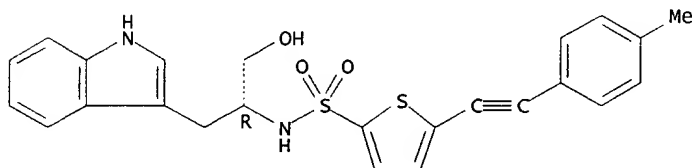
IT 251998-34-2P 251998-35-3P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of sulfonamides and TNF-.alpha. inhibitors)

RN 251998-34-2 HCAPLUS

CN 2-Thiophenesulfonamide, N-[(1R)-2-hydroxy-1-(1H-indol-3-ylmethyl)ethyl]-5-[(4-methylphenyl)ethynyl]- (9CI) (CA INDEX NAME)

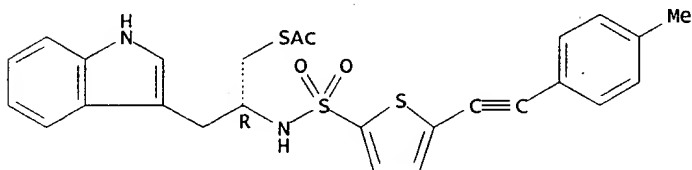
Absolute stereochemistry.



RN 251998-35-3 HCAPLUS

CN Ethanethioic acid, S-[(2R)-3-(1H-indol-3-yl)-2-[[[5-[(4-methylphenyl)ethynyl]-2-thienyl]sulfonyl]amino]propyl] ester (9CI) (CA INDEX NAME)

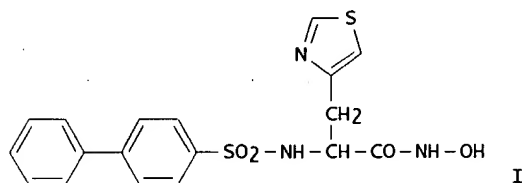
Absolute stereochemistry.



=&gt; d bib abs hitstr 164 2

L64 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1999:579153 HCAPLUS  
 DN 131:214280  
 TI Preparation of sulfonamides as MMP-8 inhibitors  
 IN Watanabe, Fumihiko; Tsumiki, Hiroshige  
 PA Shionogi and Co., Ltd., Japan  
 SO Jpn. Kokai Tokkyo Koho, 28 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 11246527	A2	19990914	JP 1998-49260	19980302
OS	MARPAT 131:214280				
GI					

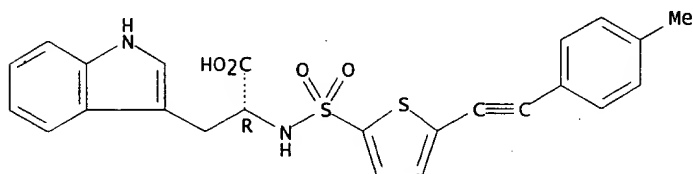


AB The title compds. R4R3SO2N(R2)CH(R1)COY [R1 = (un)substituted alkyl, etc.; R2 = H, alkyl, etc.; R3 = phenylene, etc.; R4 = (un)substituted phenyl; Y = NHOH, OH] are prepd. The title compd. I at 1000 nm gave 97.6% inhibition of MMP-8. Formulations are given.

IT 203640-27-1P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (4; prepn. of sulfonamides as MMP-8 inhibitors)

RN 203640-27-1 HCAPLUS  
 CN D-Tryptophan, N-[[5-[(4-methylphenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI)  
 (CA INDEX NAME)

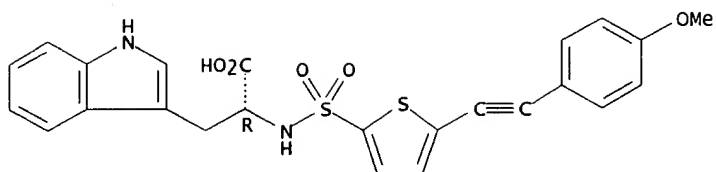
Absolute stereochemistry. Rotation (+).



IT 193809-32-4P 220043-30-1P 220043-32-3P  
 220043-34-5P 220043-40-3P 220043-41-4P  
 243144-04-9P 243144-05-0P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of sulfonamides as MMP-8 inhibitors)

RN 193809-32-4 HCAPLUS  
 CN D-Tryptophan, N-[[5-[(4-methoxyphenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI)  
 (CA INDEX NAME)

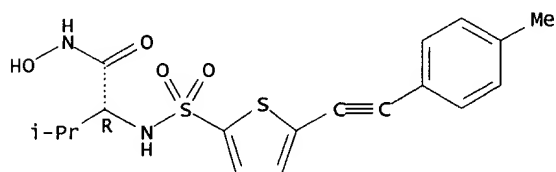
Absolute stereochemistry.



RN 220043-30-1 HCAPLUS

CN Butanamide, N-hydroxy-3-methyl-2-[[[5-[(4-methylphenyl)ethynyl]-2-thienyl]sulfonyl]amino]-, (2R)- (9CI) (CA INDEX NAME)

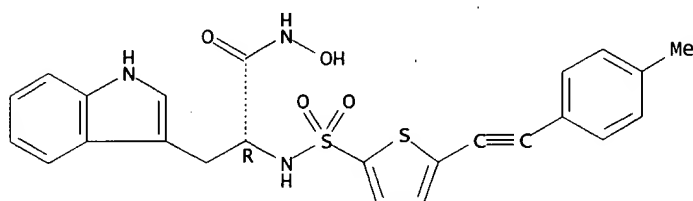
Absolute stereochemistry.



RN 220043-32-3 HCAPLUS

CN 1H-Indole-3-propanamide, N-hydroxy-.alpha.-[[[5-[(4-methylphenyl)ethynyl]-2-thienyl]sulfonyl]amino]-, (.alpha.R)- (9CI) (CA INDEX NAME)

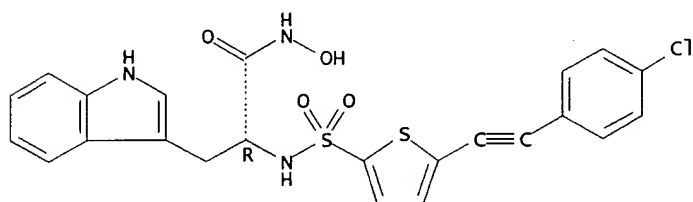
Absolute stereochemistry.



RN 220043-34-5 HCAPLUS

CN 1H-Indole-3-propanamide, .alpha.-[[[5-[(4-chlorophenyl)ethynyl]-2-thienyl]sulfonyl]amino]-N-hydroxy-, (.alpha.R)- (9CI) (CA INDEX NAME)

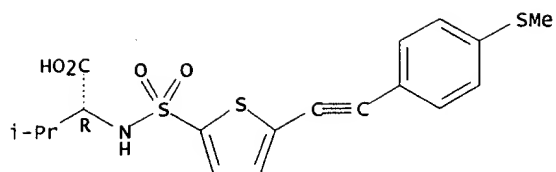
Absolute stereochemistry.



RN 220043-40-3 HCAPLUS

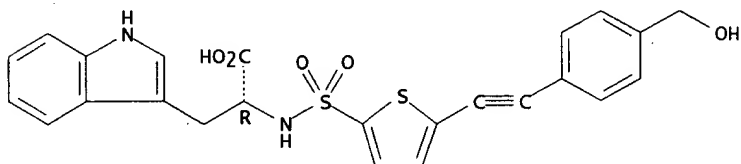
CN D-valine, N-[[[5-[[4-(methylthio)phenyl]ethynyl]-2-thienyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



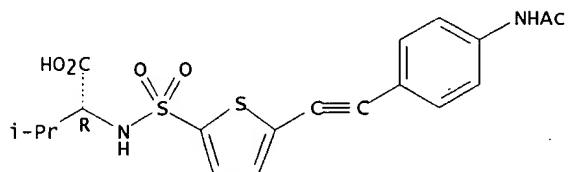
RN 220043-41-4 HCAPLUS  
 CN D-Tryptophan, N-[[5-[[4-(hydroxymethyl)phenyl]ethynyl]-2-thienyl]sulfonyl]-  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



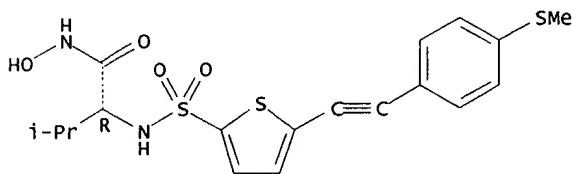
RN 243144-04-9 HCAPLUS  
 CN D-Valine, N-[[5-[[4-(acetylamino)phenyl]ethynyl]-2-thienyl]sulfonyl]-  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



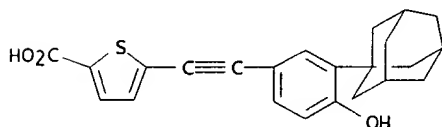
RN 243144-05-0 HCAPLUS  
 CN Butanamide, N-hydroxy-3-methyl-2-[[[5-[[4-(methylthio)phenyl]ethynyl]-2-thienyl]sulfonyl]amino]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=&gt; d bib abs hitstr 164 3

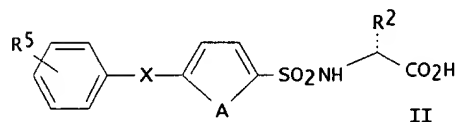
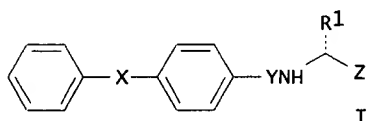
L64 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1999:455007 HCAPLUS  
 DN 131:194472  
 TI Quantitative structure-activity relationship studies of RAR .alpha.,  
 .beta., .gamma. retinoid agonists  
 AU Douguet, Dominique; Thoreau, Etienne; Grassy, Gerard  
 CS Centre International Recherches Dermatologie GALDERMA, Sophia Antipolis,  
 F-06902, Fr.  
 SO Quant. Struct.-Act. Relat. (1999), 18(2), 107-123  
 CODEN: QSARDI; ISSN: 0931-8771  
 PB Wiley-VCH Verlag GmbH  
 DT Journal  
 LA English  
 AB Structure-activity relationships were established for 140 synthetic  
 retinoid agonists. Retinoids, natural and synthetic analogs of vitamin A,  
 are activating ligands for retinoic acid receptors (RAR.alpha., .beta.,  
 and .gamma.), members of the nuclear receptor superfamily. A QSAR study  
 provides information on the type of intermol. and intramol. interactions  
 the active mols. are exposed to during the course of their interaction  
 with the receptor. Retinoid structures were modeled both by mol. and  
 quantum mechanics and were submitted to a preliminary conformational anal.  
 based on mol. dynamics. Linear and non-linear multivariate analyses were  
 performed, revealing the principal electronic and structural  
 characteristics leading to good affinity for each RAR subtype. Distinct  
 structural features were found for each subtype: this is in agreement with  
 the fact that the selectivity of the RAR subtypes results from the change  
 of amino acids in the ligand cavity. Indeed, these amino-acids induce  
 subtle changes in terms of steric properties and specific interactions,  
 thus engendering specificity. The predictive ability of these  
 relationships was validated using a large set of compds. which were not  
 used to derive the model. The goal this of work was to detect  
 relationships between structures and affinity for a broad range of  
 retinoids in order that this model could be used in a more general manner,  
 for example to impose constraints in database searching, or for use in  
 automatic structure generation software.  
 IT 173191-01-0  
 RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological  
 study); USES (Uses)  
 (QSAR studies of retinoic acid receptors .alpha., .beta., .gamma.  
 retinoid agonists)  
 RN 173191-01-0 HCAPLUS  
 CN 2-Thiophenecarboxylic acid, 5-[(4-hydroxy-3-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-  
 ylphenyl)ethynyl]- (9CI) (CA INDEX NAME)



RE.CNT 77  
 RE  
 (1) Abraham, R; J Computer Aided Mol Design 1989, V3, P175 HCAPLUS  
 (3) Anon; JP 06072866 HCAPLUS  
 (4) Bernardon, J; WO 92/06948 1991 HCAPLUS  
 (5) Bernardon, J; EP 0661258 A1 1994 HCAPLUS  
 (6) Bernardon, J; EP 0661260 A1 1994 HCAPLUS  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; d bib abs hitstr 164 4

L64 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1998:66723 HCAPLUS  
 DN 128:188290  
 TI Highly Selective and Orally Active Inhibitors of Type IV Collagenase  
 (MMP-9 and MMP-2): N-Sulfonylamino Acid Derivatives  
 AU Tamura, Yoshinori; Watanabe, Fumihiko; Nakatani, Takuji; Yasui, Ken; Fuji,  
 Masahiro; Komurasaki, Tadafumi; Tsuzuki, Hiroshige; Maekawa, Ryuji;  
 Yoshioka, Takayuki; Kawada, Kenji; Sugita, Kenji; Ohtani, Mitsuaki  
 CS Shionogi Research Laboratories, Shionogi Co. Ltd., Osaka, 553, Japan  
 SO J. Med. Chem. (1998), 41(4), 640-649  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PB American Chemical Society  
 DT Journal  
 LA English  
 GI

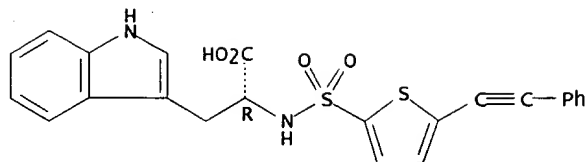


AB Various N-sulfonylamino acid derivs., e.g. I (R1 = PhCH2, X = bond, Y = SO2, CO, Z = CONHOH, CO2H; R1 = indol-3-ylmethyl, X = bond, Y = SO2, Z = CONHOH, CO2H; R1 = Me2CH, X = O, Y = SO2, Z = CONHOH, CO2H) and II (R2 = indol-3-ylmethyl, R5 = H, OMe-4, OMe-3, A = CH:CH, X = bond; R2 = indol-3-ylmethyl, R5 = Me-4, A = S, X = bond; R2 = CHMe2, R5 = OMe-4, SMe-4, A = CH:CH, X = bond; R2 = CHMe2, R5 = OMe-4, A = S, X = bond; R2 = indol-3-ylmethyl, R5 = H, Me-4, CO2H-4, A = CH:CH, X = C.tplbond.C; R2 = indol-3-ylmethyl, R5 = NO2-2, NO2-4, Me-4, A = S, X = C.tplbond.C; R2 = CHMe2, R5 = Me-4, A = CH:CH, S, X = C.tplbond.C; R2 = CH2Ph, R5 = OMe-4, A = CH:CH, S, X = C.tplbond.C), were synthesized and evaluated for their in vitro and in vivo activities to inhibit type IV collagenase (MMP-9 and MMP-2). When the amino acid residue and the sulfonamide moiety were modified, their inhibitory activities were greatly affected by the structure of the sulfonamide moiety. A series of aryl sulfonamide derivs. contg. biaryl, tetrazole, amide, and triple bond were found to be potent and highly selective inhibitors of MMP-9 and MMP-2. In addn., these compds. were orally active in animal models of tumor growth and metastasis. These results revealed the potential of the N-sulfonylamino acid derivs. as a new type of candidate drug for the treatment of cancer.

IT 193809-30-2P 193809-31-3P 193809-35-7P  
 193809-37-9P 203640-26-0P 203640-27-1P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);  
 PREP (Preparation); USES (Uses)  
 (prepn. of N-sulfonylamino acid derivs. as orally active type IV collagenase inhibitors)

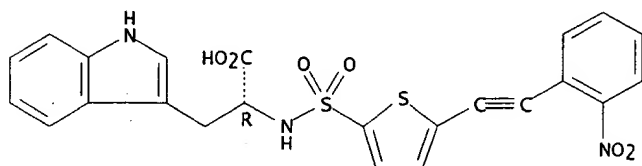
RN 193809-30-2 HCAPLUS  
 CN D-Tryptophan, N-[[5-(phenylethynyl)-2-thienyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



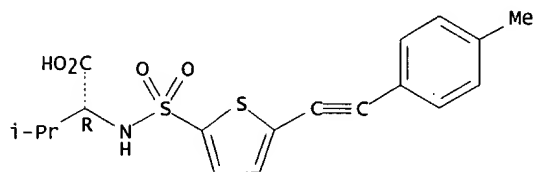
RN 193809-31-3 HCAPLUS  
 CN D-Tryptophan, N-[[5-[(2-nitrophenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



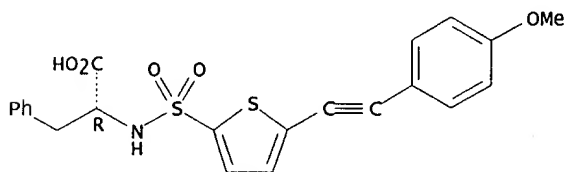
RN 193809-35-7 HCAPLUS  
 CN D-Valine, N-[[5-[(4-methylphenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI) (CA  
 INDEX NAME)

Absolute stereochemistry. Rotation (-).



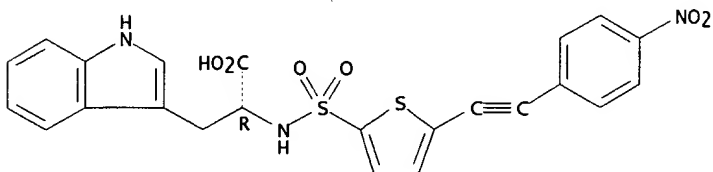
RN 193809-37-9 HCAPLUS  
 CN D-Phenylalanine, N-[[5-[(4-methoxyphenyl)ethynyl]-2-thienyl]sulfonyl]-  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 203640-26-0 HCAPLUS  
 CN D-Tryptophan, N-[[5-[(4-nitrophenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



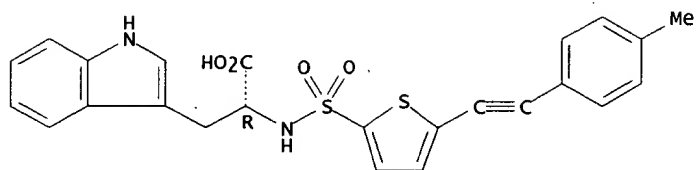
RN 203640-27-1 HCAPLUS  
 CN D-Tryptophan, N-[[5-[(4-methylphenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI)

SEARCHED BY SUSAN HANLEY 305-4053

CHOI 09/387,135

(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).





=&gt; d bib abs hitstr 164 5

L64 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2001 ACS

AN 1997:231462 HCAPLUS

DN 126:317376

TI Preparation of substituted arylalkynyl- and heteroarylalkynyl-N-hydroxyureas as inhibitors of leukotriene biosynthesis

IN Basha, Anwer; Brooks, Clint D. W.; Bhatia, Pramila; Craig, Richard A.; Ratajczyk, James D.; Stewart, Andrew O.

PA Abbott Laboratories, USA

SO U.S., 25 pp. Cont.-in-part of U.S. 5,288,751.

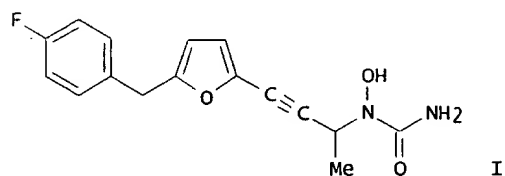
CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5616596	A	19970401	US 1995-416807	19950413
	US 5288751	A	19940222	US 1992-973100	19921106
	WO 9411342	A1	19940526	WO 1993-US10675	19931105
	W: AU, CA, JP, KR, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRAI	US 1992-973100		19921106		
	WO 1993-US10675		19931105		
OS	MARPAT 126:317376				
GI					



AB The title compds. A-L-Z-C.tplbond.C-B-N(OM)C(O)NH<sub>2</sub> [M = H, a pharmaceutically acceptable cation, a pharmaceutically acceptable metabolically cleavable group; B = C1-12 divalent alkylene; Z = (un)substituted thiazolyl, furyl, thienyl; L = C1-6 alkylene, C2-6 alkynylene, C(O), etc.; A = (un)substituted carbocyclic aryl], having activity to inhibit lipoxygenase, were prepd. Thus, reaction of 4-[5-(4-fluorophenylmethyl)furyl-2-yl]-3-butyne-2-ol with N,O-bis-phenyloxycarbonylhydroxylamine in the presence of Ph<sub>3</sub>P and diisopropyl azodicarboxylate in THF followed by ammonolysis of the resulting N,O-bis(phenyloxycarbonyl)-N-{3-[5-(4-fluorophenylmethyl)furyl-2-yl]-1-methyl-2-propynyl}hydroxylamine afforded I which showed IC<sub>50</sub> of 0.06 .mu.M against stimulated LTB<sub>4</sub> formation in human whole blood.

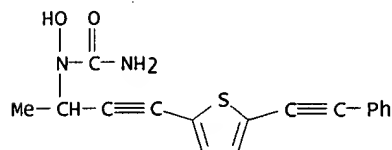
IT 154355-67-6P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of substituted arylalkynyl- and heteroarylalkynyl-N-hydroxyureas as inhibitors of leukotriene biosynthesis)

RN 154355-67-6 HCAPLUS

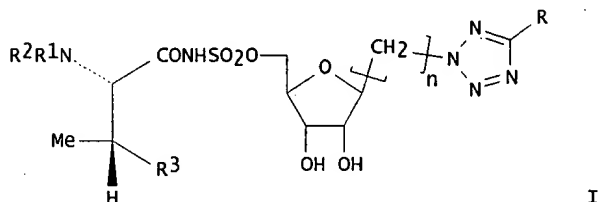
CN Urea, N-hydroxy-N-[1-methyl-3-[5-(phenylethynyl)-2-thienyl]-2-propynyl]-(9CI) (CA INDEX NAME)



=&gt; d bib abs hitstr 164 6

L64 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1997:231091 HCAPLUS  
 DN 126:212376  
 TI Preparation of aminoacyl adenylate mimics as novel antimicrobial and antiparasitic agents  
 IN Hill, Jason M.; Yu, Guixue; Shue, Youe-Kong; Zydowsky, Thomas M.; Rebek, Julius, Jr.  
 PA Cubist Pharmaceuticals, Inc., USA  
 SO PCT Int. Appl., 57 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9705132	A1	19970213	WO 1996-US11910	19960718
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN				
	US 5726195	A	19980310	US 1996-683809	19960716
	AU 9665006	A1	19970226	AU 1996-65006	19960718
PRAI	US 1995-1649		19950728		
	US 1996-14881		19960404		
	US 1996-683809		19960716		
	WO 1996-US11910		19960718		
OS	MARPAT 126:212376				
GI					



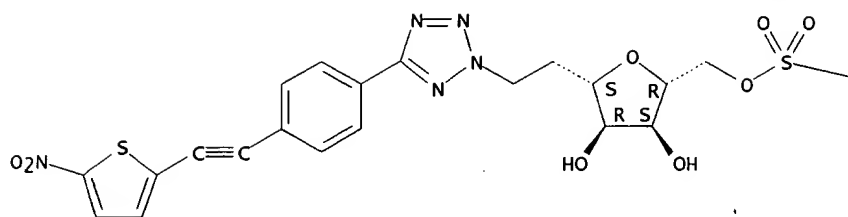
AB Aminoacyl adenylate mimics I (R = amino, alkyl, aryl, cycloalkyl, alkoxy, aryloxy; R1, R2 = alkyl, aryl, carboalkoxy; alkylthiocarbonyl, carboxamido, acyl; R3 = Et, OMe; n = 1, 2) are described. An exemplary compd. of this invention is [S-(R\*, R\*)]-3,6-anhydro-1,2-dideoxy-1-[5-[4-[(5-nitro-2-thienyl)ethynyl]phenyl]-2H-tetrazol-2-yl]-D-allo-heptitol 7-(2-amino-3-methyl-1-oxopentyl)sulfamate. These compds. inhibit isoleucyl-tRNA synthetases and are useful as antimicrobial and antiparasitic agents such as multi-drug resistant Streptococcus pyogenes (IC50 = 0.3-11 nM).

IT 188022-36-8P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);  
 PREP (Preparation); USES (Uses)  
 (prepn. of aminoacyl adenylate mimics as novel antimicrobial and antiparasitic agents)

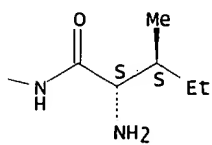
RN 188022-36-8 HCAPLUS  
 CN D-allo-Heptitol, 3,6-anhydro-1,2-dideoxy-1-[5-[4-[(5-nitro-2-thienyl)ethynyl]phenyl]-2H-tetrazol-2-yl]-, 7-[[[(2S,3S)-2-amino-3-methyl-1-oxopentyl]sulfamate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



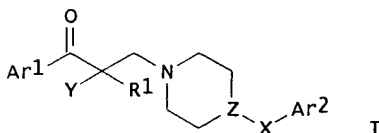
PAGE 1-B



=&gt; d bib abs hitstr 164 7

L64 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1996:476743 HCAPLUS  
 DN 125:142771  
 TI Preparation of 1-aryl-3-piperazinopropanones for treatment of Alzheimer's disease  
 IN Debernardis, John F.; Kerkman, Daniel J.; Zinkowski, Raymond P.  
 PA Molecular Geriatrics Corporation, USA  
 SO PCT Int. Appl., 113 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9616052	A2	19960530	WO 1995-US14987	19951116
	WO 9616052	A3	19960801		
	W:	AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT			
	RW:	KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
	US 5693804	A	19971202	US 1994-341507	19941117
	AU 9642387	A1	19960617	AU 1996-42387	19951116
	AU 711703	B2	19991021		
	EP 792269	A2	19970903	EP 1995-940734	19951116
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE			
	JP 10510248	T2	19981006	JP 1995-516990	19951116
PRAI	US 1994-341507		19941117		
	WO 1995-US14987		19951116		
OS	MARPAT 125:142771				
GI					

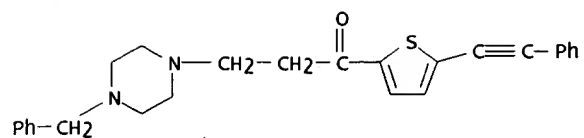


AB The title compds., [I; X = CO, SO<sub>2</sub>, CH<sub>2</sub>, CHPh; Z = N, CH; Ar1 = (substituted) Ph; thienyl, furyl, etc.; Ar2 = naphthyl, thienyl, furyl, etc.; Y = H, bonded to Ar1 through CH<sub>2</sub>, etc.; R1 = H, alkyl, (substituted) Ph], useful in the treatment of neoplastic diseases, and bacterial or fungal infections, and in preventing or decreasing the prodn. of abnormally phosphorylated paired helical filament (PHF) epitopes assocd. with Alzheimer's Disease, were prepd. Reaction of 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>COME with 1-benzylpiperazine and paraformaldehyde in the presence of conc. HCl in i-PROH afforded I.2HCl [X = CH<sub>2</sub>; Z = N; Ar1 = 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>; Ar2 = Ph; Y = R1 = H] which showed IC<sub>50</sub> of 5.0 .mu.M for inhibition TG3 immunoreactivity in OKA (okadaic acid) treated MSN1a cells.

IT 179335-34-3P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);  
 PREP (Preparation); USES (Uses)  
 (prepn. of 1-aryl-3-piperazinopropanones for treatment of Alzheimer's disease)

RN 179335-34-3 HCAPLUS  
 CN 1-Propanone, 1-[5-(phenylethynyl)-2-thienyl]-3-[4-(phenylmethyl)-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)

CHOI 09/387,135

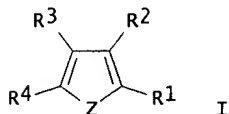


● 2 HCl

=&gt; d bib abs hitstr 164 8

L64 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1995:994741 HCAPLUS  
 DN 124:86809  
 TI Preparation of (pyrrolyl- and thienylcarbonyl)guanidines as  
 sodium-hydrogen exchange inhibitors, antiarrhythmic agents, and cell  
 proliferation inhibitors  
 IN Kleemann, Heinz-Werner; Lang, Hans-Jochen; Schwark, Jan-Robert; Weichert,  
 Andreas; Scholz, Wolfgang; Albus, Udo  
 PA Hoechst A.-G., Germany  
 SO Eur. Pat. Appl., 48 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA German  
 FAN.CNT 1

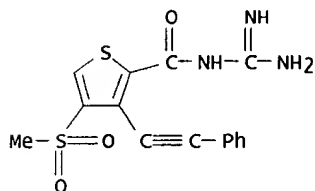
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 676395	A2	19951011	EP 1995-105088	19950405
	EP 676395	A3	19960306		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	DE 4412334	A1	19951019	DE 1994-4412334	19940411
	FI 9501681	A	19951012	FI 1995-1681	19950407
	AU 9516354	A1	19951019	AU 1995-16354	19950407
	AU 683722	B2	19971120		
	US 5698581	A	19971216	US 1995-418434	19950407
	CA 2146707	AA	19951012	CA 1995-2146707	19950410
	NO 9501405	A	19951012	NO 1995-1405	19950410
	JP 07291927	A2	19951107	JP 1995-107811	19950410
	ZA 9502930	A	19960126	ZA 1995-2930	19950410
	HU 71616	A2	19960129	HU 1995-1035	19950410
	CN 1117044	A	19960221	CN 1995-104391	19950410
PRAI	DE 1994-4412334		19940411		
OS	MARPAT 124:86809				
GI					



AB Title compds. [I; 1 of R1,R2 = CON:C(NH2)2 and the other = H, halo, alkyl, CON:C(NH2)2, NH2, etc.; R3,R4 = H, halo, cyano, alkyl, Ph, heteroaryl, etc.; Z = SO0-2, O, NR5; R5 = H, alkyl, etc.] were prepd. Thus, Me 1-methylpyrrole-2-carboxylate was alkylated with (CF3)2CFI and the product amidated with guanidine to give I [R1 = CON:C(NH2)2, R2 = R3 = H, R4 = (CF3)2CF, Z = NMe] which ad IC50 of 0.3.mu.M against Na+/H+ exchange in rabbit erythrocytes in vitro.

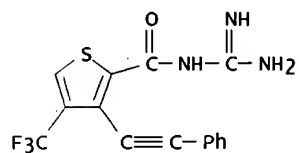
IT 172457-85-1P 172461-16-4P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of (pyrrolyl- and thienylcarbonyl)guanidines as sodium-hydrogen exchange inhibitors, antiarrhythmic agents, and cell proliferation inhibitors)

RN 172457-85-1 HCAPLUS  
 CN 2-Thiophenecarboxamide, N-(aminoiminomethyl)-4-(methylsulfonyl)-3-(phenylethynyl)- (9CI) (CA INDEX NAME)



CHOI 09/387,135

RN 172461-16-4 HCAPLUS  
CN 2-Thiophenecarboxamide, N-(aminoiminomethyl)-3-(phenylethynyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



=&gt; d bib abs hitstr 164 9

L64 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2001 ACS

AN 1994:244653 HCAPLUS

DN 120:244653

TI Preparation of N-[(phenylalkyl)furylalkynyl]- and - thienylalkynyl]-N-hydroxyureas and analogs as inhibitors of leukotriene biosynthesis

IN Brooks, Dee W.; Stewart, Andrew O.; Basha, Anwer; Bhatia, Pramila; Ratajczyk, James D.

PA Abbott Laboratories, USA

SO U.S., 15 pp.

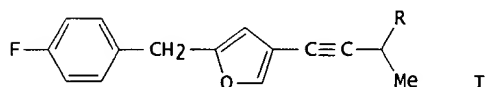
CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5288751	A	19940222	US 1992-973100	19921106
	WO 9411342	A1	19940526	WO 1993-US10675	19931105
	W: AU, CA, JP, KR, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2136077	AA	19940526	CA 1993-2136077	19931105
	AU 9456660	A1	19940608	AU 1994-56660	19931105
	AU 673040	B2	19961024		
	EP 667855	A1	19950823	EP 1994-902209	19931105
	EP 667855	B1	19990324		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	JP 08503200	T2	19960409	JP 1993-511496	19931105
	AT 178049	E	19990415	AT 1994-902209	19931105
	ES 2131185	T3	19990716	ES 1994-902209	19931105
	US 5616596	A	19970401	US 1995-416807	19950413
PRAI	US 1992-973100		19921106		
	WO 1993-US10675		19931105		
OS	MARPAT 120:244653				
GI					



AB ALZC.tplbond.CBN(OM)CONH2 [A = (substituted) carbocyclic aryl; B = alkylene; L = (O- or CO-interrupted)alkylene, CO, C(:NOH), etc.; M = H, cation, metabolically labile group; Z = phenylene, furylene, thienylene, etc.] were prepd. Thus, 4-FC6H4CH2Br was condensed with furan and the brominated product condensed with HC.tplbond.CCH(OH)Me to give butynol I (R = OH) which was condensed with PhO2CNHOCO2Ph to give, after aq. NH3 treatment, I [R = N(OH)CONH2]. The latter gave 68% inhibition of leukotriene biosynthesis in a rat peritoneal anaphylaxis model at 30.mu.mol/kg orally.

IT 154355-67-6P

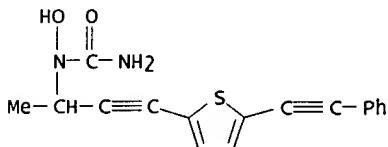
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);

PREP (Preparation); USES (Uses)

(prepn. of, as leukotriene biosynthesis inhibitor)

RN 154355-67-6 HCAPLUS

CN Urea, N-hydroxy-N-[1-methyl-3-[5-(phenylethynyl)-2-thienyl]-2-propynyl]-(9CI) (CA INDEX NAME)

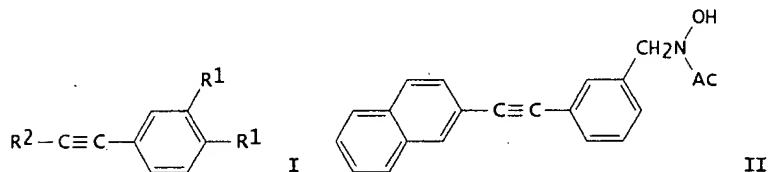




=&gt; d bib abs hitstr 164 10

L64 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1992:426103 HCAPLUS  
 DN 117:26103  
 TI Lipoxxygenase-inhibiting substituted phenylacetylenes, pharmaceuticals containing them, and methods for the preparation of the compounds and pharmaceuticals  
 IN Zimmer, Oswald; Vollenberg, Werner; Seipp, Ulrich; Englberger, Werner; Haurand, Michael; Bosman, Brigitte J.; Schneider, Johannes  
 PA Gruenenthal G.m.b.H., Germany  
 SO Eur. Pat. Appl., 40 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA German  
 FAN.CNT 1

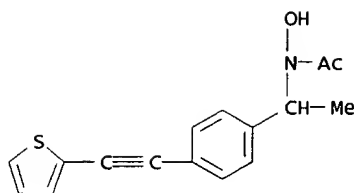
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 468281	A1	19920129	EP 1991-111487	19910710
	EP 468281	B1	19950308		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	DE 4023742	A1	19920130	DE 1990-4023742	19900726
	CA 2043823	AA	19920127	CA 1991-2043823	19910604
	IL 98391	A1	19950526	IL 1991-98391	19910606
	ZA 9104386	A	19920429	ZA 1991-4386	19910607
	HU 58047	A2	19920128	HU 1991-2296	19910708
	AU 9180333	A1	19920130	AU 1991-80333	19910710
	AU 637513	B2	19930527		
	ES 2072487	T3	19950716	ES 1991-111487	19910710
	US 5202349	A	19930413	US 1991-732168	19910718
	FI 9103565	A	19920127	FI 1991-3565	19910725
	JP 04243856	A2	19920831	JP 1991-186444	19910725
	RU 2014323	C1	19940615	RU 1991-5001103	19910725
PRAI	DE 1990-4023742		19900726		
OS	MARPAT 117:26103				
GI					



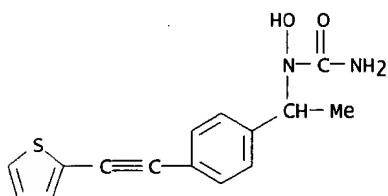
AB Title compds. I [one of R1 = H, the other = CHR3N(OH)COR4; R2 = certain (un)substituted Ph, naphthyl, thienyl, benzothienyl, pyridyl, quinoliny, or benzodioxolanyl; R3 = H, Me, Et; R4 = Me, amino] were prepd. as selective lipoxxygenase inhibitors, useful esp. as antiasthmatics. For example, coupling of naphth-2-ylacetylene and 3-bromobenzaldehyde using (Ph3P)2PdCl2 and CuI catalysts in Et3N gave 65.5% 3-(naphth-2-ylethynyl)benzaldehyde, which underwent oximation (97.2%), followed by redn. of the oxime with NaBH3CN and acetylation with Ac2O (62.6%) to give title compd. II. In vitro tests of II showed IC50 values of 0.67 .mu.M and >500 .mu.M for inhibition of 5-lipoxxygenase and cyclooxygenase, resp. Preps. of over 60 I are described, along with addnl. biol. data for some.

IT 141697-19-0P 141697-20-3P 141697-21-4P  
 141697-22-5P 141697-23-6P 141697-24-7P  
 141697-25-8P 141697-26-9P 141697-27-0P  
 141697-28-1P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of, as lipoxxygenase inhibitor)

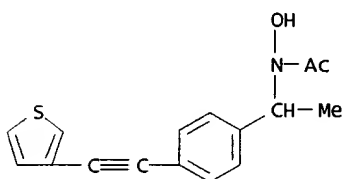
RN 141697-19-0 HCAPLUS  
 CN Acetamide, N-hydroxy-N-[1-[4-(2-thienylethynyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)



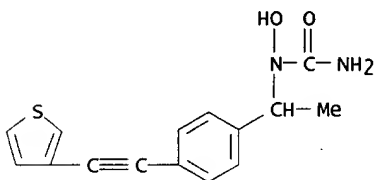
RN 141697-20-3 HCAPLUS  
CN Urea, N-hydroxy-N-[1-[4-(2-thienylethynyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)



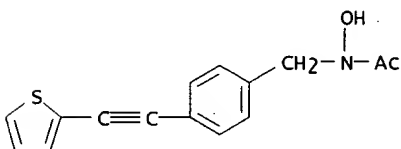
RN 141697-21-4 HCAPLUS  
CN Acetamide, N-hydroxy-N-[1-[4-(3-thienylethynyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)



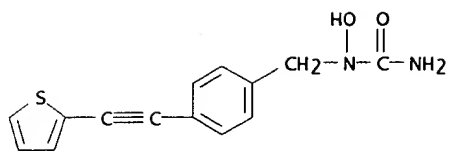
RN 141697-22-5 HCAPLUS  
CN Urea, N-hydroxy-N-[1-[4-(3-thienylethynyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)



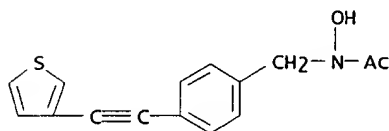
RN 141697-23-6 HCAPLUS  
CN Acetamide, N-hydroxy-N-[[4-(2-thienylethynyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



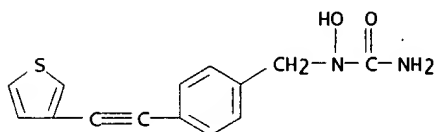
RN 141697-24-7 HCAPLUS  
CN Urea, N-hydroxy-N-[[4-(2-thienylethynyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



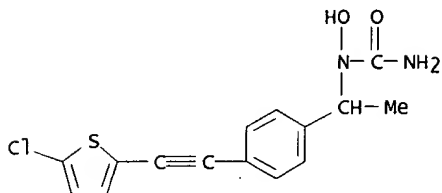
RN 141697-25-8 HCAPLUS  
 CN Acetamide, N-hydroxy-N-[[4-(3-thienylethynyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



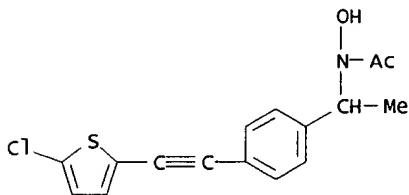
RN 141697-26-9 HCAPLUS  
 CN Urea, N-hydroxy-N-[[4-(3-thienylethynyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



RN 141697-27-0 HCAPLUS  
 CN Urea, N-[1-[4-[(5-chloro-2-thienyl)ethynyl]phenyl]ethyl]-N-hydroxy- (9CI) (CA INDEX NAME)

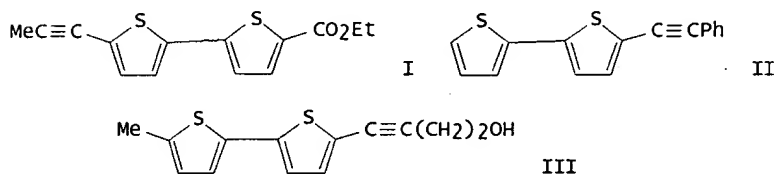


RN 141697-28-1 HCAPLUS  
 CN Acetamide, N-[1-[4-[(5-chloro-2-thienyl)ethynyl]phenyl]ethyl]-N-hydroxy- (9CI) (CA INDEX NAME)



=&gt; d bib abs hitstr 164 11

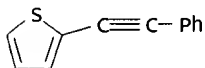
L64 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1989:185340 HCAPLUS  
 DN 110:185340  
 TI Antiviral properties of acetylenes and thiophenes  
 AU Hudson, J. B.; Towers, G. H. N.  
 CS Dep. Bot., Univ. British Columbia, Vancouver, BC, Can.  
 SO Bioact. Mol. (1988), 7 (Chem. Biol. Nat.-Occurring Acetylenes Relat. Compd.), 315-38  
 CODEN: BMOLEY; ISSN: 0921-0687  
 DT Journal  
 LA English  
 GI



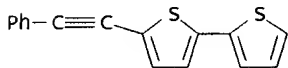
AB A series of 31 synthetic thiophenes was tested for antiviral activity in vitro using Sindbis virus or murine cytomegalovirus infection of murine 3T3-L1 cells and std. UV-A exposure as the test system. None of the compds. were active in the dark. I was the most potent inhibitor of Sindbis virus, and II and III were the most active against murine cytomegalovirus. In general, there was a fairly good agreement between the results for the 2 viruses. Structure-activity relationships are discussed. The antiviral activities of 5 addnl. compds. (thiarubrine A, thiophene A, .alpha.-terthienyl, phenylheptatriyne, and ACBP-thiophene) are reviewed.

IT 4805-17-8 4805-21-4 90267-18-8  
 RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (virucidal activity of, light-dependent, structure in relation to)

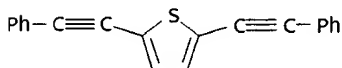
RN 4805-17-8 HCAPLUS  
 CN Thiophene, 2-(phenylethynyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 4805-21-4 HCAPLUS  
 CN 2,2'-Bithiophene, 5-(phenylethynyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 90267-18-8 HCAPLUS  
 CN Thiophene, 2,5-bis(phenylethynyl)- (9CI) (CA INDEX NAME)



=&gt; d bib abs hitstr 164 12

L64 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2001 ACS

AN 1987:617636 HCAPLUS

DN 107:217636

TI Preparation of 1,1-disubstituted cyclopropane derivatives as medical fungicides

IN Ehrhardt, Heinz; Blume, Ernst; Raether, Wolfgang; Dittmar, Walter

PA Hoechst A.-G., Fed. Rep. Ger.

SO Ger. Offen., 26 pp.

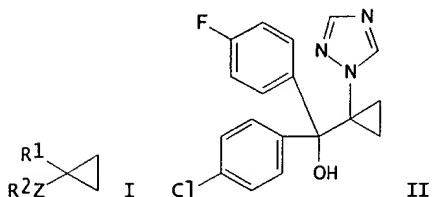
CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3608727	A1	19870917	DE 1986-3608727	19860315
	EP 237916	A2	19870923	EP 1987-103390	19870310
	EP 237916	A3	19900822		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	FI 8701080	A	19870916	FI 1987-1080	19870312
	DK 8701313	A	19870916	DK 1987-1313	19870313
	NO 8701051	A	19870916	NO 1987-1051	19870313
	NO 165104	B	19900917		
	NO 165104	C	19901227		
	AU 8769990	A1	19870917	AU 1987-69990	19870313
	AU 588980	B2	19890928		
	JP 62230742	A2	19871009	JP 1987-56944	19870313
	ZA 8701838	A	19871028	ZA 1987-1838	19870313
	HU 43829	A2	19871228	HU 1987-1106	19870313
	US 4829075	A	19890509	US 1987-25581	19870313
IL 81880	A1	19910131	IL 1987-81880	19870313	
NO 8703865	A	19870916	NO 1987-3865	19870915	
PRAI	DE 1986-3608727		19860315		
GI	NO 1987-1051		19870313		



AB The title compds. [I; R1 = pyrrolidinyl, piperidinyl, morpholino, amino, (substituted) alkoxy, alkylthio, benzothiazolyloxy, etc.; R2 = Me3C, (substituted) Ph, biphenyl, phenylsulfonylphenyl, naphthyl, indanyl, etc.; Z = CH2, C:O, C:R3H, C:NNR4H, C:NOR5, COR5R6; R3 = CN, H, (substituted) alkyl, cycloalkyl, C6H5CO, Ph; R4 = H, alkyl, (substituted) Ph; R5 = H, (substituted) alkyl, cycloalkyl, alkenyl, alkynyl, farnesyl, triazolylmethyl, Ph, etc.; R6 = H, alkyl, alkynyl, (substituted) phenylethynyl, PhCH2, Ph] were prepd. as medical fungicides. 4-chlorophenyl-1-(1,2,4-triazol-1-yl)cyclopropyl ketone in THF was added to 4-FC6H4MgBr in Et2O at room temp. and the mixt. was refluxed 2 h to give 73% triazolylcyclopropylcarbinol II. In mice infected with *Candida albicans* 8 times. 30 mg II/kg orally increased survival times by 48% over those of animals treated with ketoconazole.

IT 111262-80-7P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of, as medical fungicide)

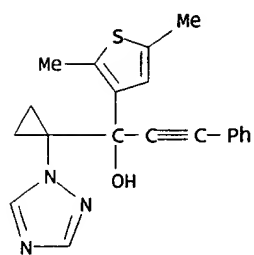
RN 111262-80-7 HCAPLUS

CN 3-Thiophenemethanol, 2,5-dimethyl-.alpha.-(phenylethynyl)-.alpha.-[1-(1H-1,2,4-triazol-1-yl)cyclopropyl]-, mononitrate (salt) (9CI) (CA INDEX NAME)

CM 1

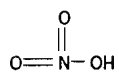
CHOI 09/387,135

CRN 111262-79-4  
CMF C20 H19 N3 O S



CM 2

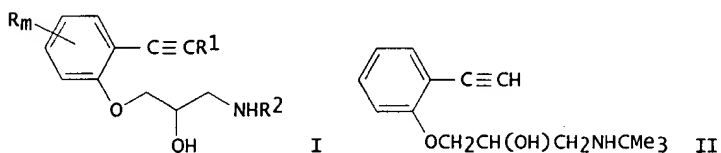
CRN 7697-37-2  
CMF H N O3



=&gt; d bib abs hitstr 164 13

L64 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1987:477423 HCAPLUS  
 DN 107:77423  
 TI Preparation of heteroaromatic acetylenes useful as antihypertensive agents  
 IN Carson, John R.  
 PA McNeilab, Inc., USA  
 SO U.S., 8 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4663334	A	19870505	US 1985-807551	19851211
	US 4728666	A	19880301	US 1986-934371	19861124
	CA 1292739	A1	19911203	CA 1986-524856	19861209
	FI 8605028	A	19870612	FI 1986-5028	19861210
	DK 8605946	A	19870612	DK 1986-5946	19861210
	NO 8604987	A	19870612	NO 1986-4987	19861210
	EP 226447	A2	19870624	EP 1986-309601	19861210
	EP 226447	A3	19880831		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 62175460	A2	19870801	JP 1986-292673	19861210
	ZA 8609333	A	19880727	ZA 1986-9333	19861210
	CN 86108922	A	19870805	CN 1986-108922	19861211
	HU 44013	A2	19880128	HU 1986-5174	19861211
	HU 196373	B	19881128		
AU 8666424	A1	19880616	AU 1986-66424	19861211	
AU 597319	B2	19900531			
PRAI	US 1985-807551		19851211		
GI					

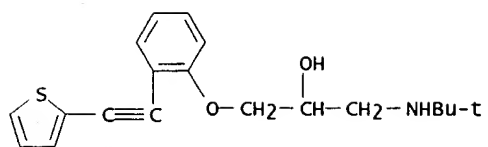


AB Title compds. I [R = alkyl, alkoxy, halo, alkoxyalkyl, carboxamidoalkyl, Cl, F, Br; m = 0-2; R1 = (un)substituted heterocycyl; R2 = C3-7 alkyl], useful as antihypertensives, are prepd. A THF/Et3N soln. of 6.1 g ethynylphenoxypropanolamine II was coupled with 5.8 g 4-bromopyridine in the presence of 0.14 g (Ph3P)4Pd and 0.05 g CuI over 18 h under a N atm. to give I (m = 0, R1 = 4-pyridinyl, R2 = CMe3), isolated as the fumarate salt. This compd. at 30 mg/kg orally caused a 46 mm Hg drop in blood pressure (sustained for 7.5 h) in std. spontaneously hypertensive rat testing.

IT 109684-33-5P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);  
 PREP (Preparation); USES (Uses)  
 (prepn. of, as antihypertensive)

RN 109684-33-5 HCAPLUS  
 CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-[2-(2-thienylethynyl)phenoxy]-, hydrochloride (9CI) (CA INDEX NAME)

CHOI 09/387,135



● HCl



=&gt; d bib abs hitstr 163 12

L63 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2001 ACS

AN 1998:764185 HCAPLUS

DN 130:24857

TI Preparation of [(biphenyl)butenynyl]benzoates and analogs as retinoid receptor ligands

IN Bernardon, Jean-michel; Nedoncelle, Philippe

PA Centre International De Recherches Dermatologiques Galderma (C.I.R.D. Galder, Fr.

SO Eur. Pat. Appl., 72 pp.

CODEN: EPXXDW

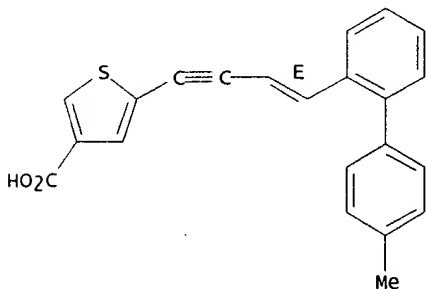
DT Patent

LA French

FAN.CNT 1

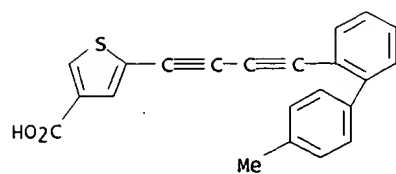
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 879814	A1	19981125	EP 1998-401144	19980513
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
FR 2763588	A1	19981127	FR 1997-6340	19970523
FR 2763588	B1	19990709		
AU 9867049	A1	19981126	AU 1998-67049	19980519
AU 713781	B2	19991209		
NO 9802296	A	19981124	NO 1998-2296	19980520
ZA 9804296	A	19981126	ZA 1998-4296	19980521
CA 2238465	AA	19981123	CA 1998-2238465	19980522
JP 11029522	A2	19990202	JP 1998-141929	19980522
JP 2974658	B2	19991110		
BR 9802130	A	19990720	BR 1998-2130	19980525
US 6150413	A	20001121	US 1998-84235	19980526 <--
PRAI FR 1997-6340		19970523		
OS MARPAT 130:24857				
AB R1Z1Z2Z3R3 [I; R1 = Me, CH2OH, OH, CHO, CO2H, etc.; R3 = (un)substituted Ph, -pyridyl, -thienyl, -furyl, etc.; Z1 = (un)substituted 1,4-phenylene, -pyridinediyl, -furandiyl, -thiophenediyl; Z2 = (E)-CR7:CHC.tplbond.C, (E,E)-CR7:CHCR8:CH, (E)-CR7:CHCONR9, etc.; R7-R9 = H or alkyl; Z3 = (un)substituted phenylene] were prepd. Thus, 2-PhC6H4CH:CHI was condensed with 4-(HC.tplbond.C)C6H4CO2Me (prepn. each given) to give, after sapon., (E)-2-PhC6H4CH:CHC.tplbond.CC6H4(CO2H)-4. Data for biol. activity of I were given.				
IT 216442-32-9P 216442-43-2P				
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)				
(prepn. of [(biphenyl)butenynyl]benzoates and analogs as retinoid receptor ligands)				
RN 216442-32-9	HCAPLUS			
CN 3-Thiophenecarboxylic acid, 5-[4-(4'-methyl[1,1'-biphenyl]-2-yl)-1,3-buten-1-ynyl]- (9CI)	(CA INDEX NAME)			

Double bond geometry as shown.



RN 216442-43-2 HCAPLUS

CN 3-Thiophenecarboxylic acid, 5-[4-(4'-methyl[1,1'-biphenyl]-2-yl)-1,3-buten-1-ynyl]- (9CI) (CA INDEX NAME)



RE.CNT 5

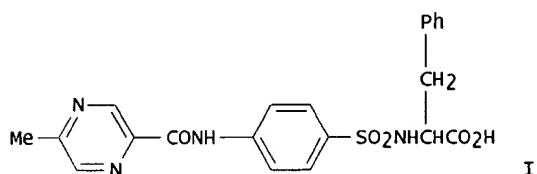
RE

- (1) Chandraratna, R; European Journal of Medicinal Chemistry Chimica  
Therapeutica 1995, V30, P505s HCAPLUS
- (2) Hisamitsu Pharmaceutical Co Inc Jp; JP 61271262 A HCAPLUS
- (3) Jong, L; Journal of Medicinal Chemistry 1993, V36(18) HCAPLUS
- (4) Kagechika, H; Journal of Medicinal Chemistry 1988, V31(11), P2182 HCAPLUS
- (5) Torrado, A; Synthesis 1995, P285 HCAPLUS

=&gt; d bib abs hitstr 163 13

L63 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1997:513624 HCAPLUS  
 DN 127:162119  
 TI Preparation of N-sulfonylamino acid derivatives as metalloproteinase inhibitors  
 IN Watanabe, Fumihiko; Tsuzuki, Hiroshige; Ohtani, Mitsuaki  
 PA Shionogi and vCo., Ltd., Japan; Watanabe, Fumihiko; Tsuzuki, Hiroshige; Ohtani, Mitsuaki  
 SO PCT Int. Appl., 128 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9727174	A1	19970731	WO 1997-JP126	19970122
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2242416	AA	19970731	CA 1997-2242416	19970122
	AU 9713195	A1	19970820	AU 1997-13195	19970122 <--
	AU 715764	B2	20000210		
	CN 1214041	A	19990414	CN 1997-193226	19970122
	BR 9707010	A	19990720	BR 1997-7010	19970122
	EP 950656	A1	19991020	EP 1997-900747	19970122
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	NO 9803376	A	19980914	NO 1998-3376	19980722
	US 6150394	A	20001121	US 1998-120378	19980722 <--
PRAI	JP 1996-30082		19960123		
	JP 1996-213555		19960813		
	WO 1997-JP126		19970122		
OS	MARPAT 127:162119				
GI					



AB The title compds. R5R4R3SO2NR2CHR1COY [R1 = (un)substituted alkyl, aryl, aralkyl, heteroaryl, etc.; R2 = H, (un)substituted alkyl, etc.; R3 = single bond, (un)substituted arylene, etc.; R4 = single bond, CH:CH, C.tplbond.C, CO, CONH, N:N, NHCONH, NHCO, O, S, SO2NH, etc.; R5 = (un)substituted alkyl, cycloalkyl, etc.; Y = NHOH, OH; a proviso is given] are prepd. The title compd. (R)-I in vitro showed IC50 of 3.95 .mu.M against MMP-9 (gelatinase B).

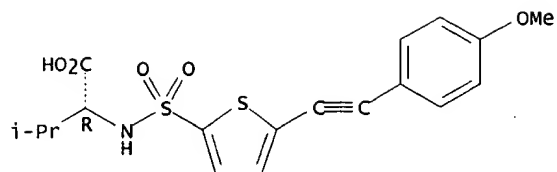
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 193809-32-4P 193809-33-5P 193809-34-6P  
 193809-35-7P 193809-36-8P 193809-37-9P  
 193809-38-0P 193809-39-1P 193809-40-4P  
 193809-41-5P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of sulfonylamino acid derivs. as metalloproteinase inhibitors)

RN 193809-07-3 HCAPLUS  
 CN D-Valine, N-[[5-[(4-methoxyphenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI) (CA INDEX NAME)

SEARCHED BY SUSAN HANLEY 305-4053

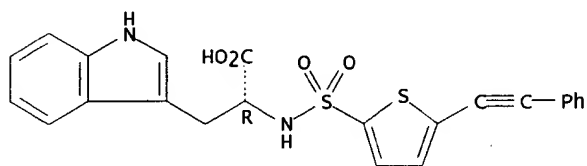
Page 3

Absolute stereochemistry.



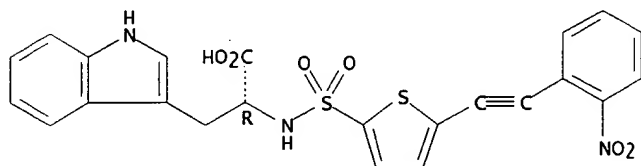
RN 193809-30-2 HCAPLUS  
 CN D-Tryptophan, N-[[5-(phenylethynyl)-2-thienyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



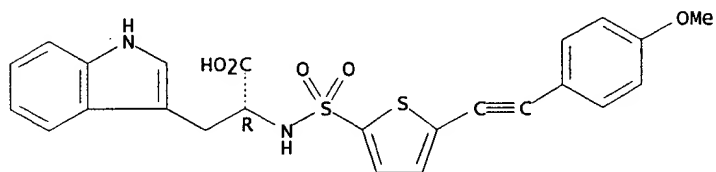
RN 193809-31-3 HCAPLUS  
 CN D-Tryptophan, N-[[5-[(2-nitrophenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



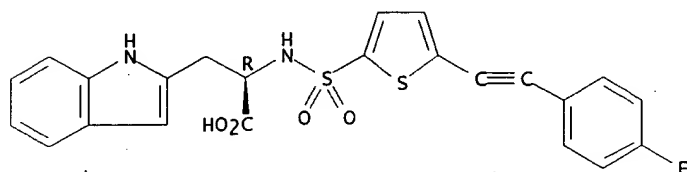
RN 193809-32-4 HCAPLUS  
 CN D-Tryptophan, N-[[5-[(4-methoxyphenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



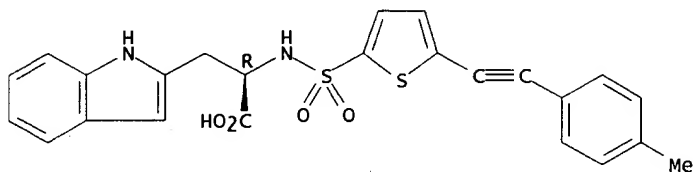
RN 193809-33-5 HCAPLUS  
 CN 1H-Indole-2-propanoic acid, .alpha.-[[[5-[(4-fluorophenyl)ethynyl]-2-thienyl]sulfonyl]amino]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



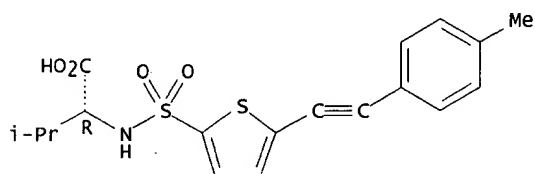
RN 193809-34-6 HCAPLUS  
 CN 1H-Indole-2-propanoic acid, .alpha.-[[[5-[(4-methylphenyl)ethynyl]-2-thienyl]sulfonyl]amino]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



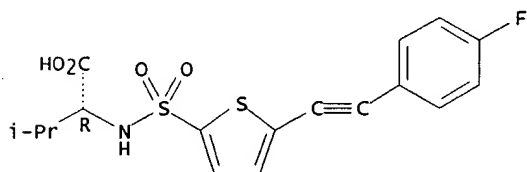
RN 193809-35-7 HCAPLUS  
 CN D-Valine, N-[[[5-[(4-methylphenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



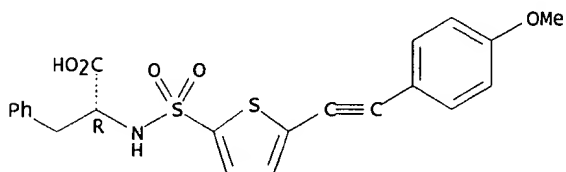
RN 193809-36-8 HCAPLUS  
 CN D-Valine, N-[[[5-[(4-fluorophenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



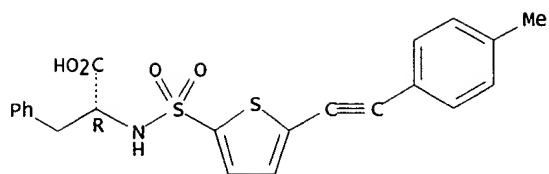
RN 193809-37-9 HCAPLUS  
 CN D-Phenylalanine, N-[[[5-[(4-methoxyphenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



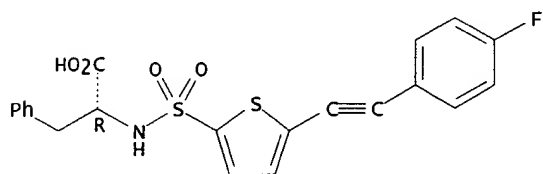
RN 193809-38-0 HCAPLUS  
 CN D-Phenylalanine, N-[[[5-[(4-methylphenyl)ethynyl]-2-thienyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



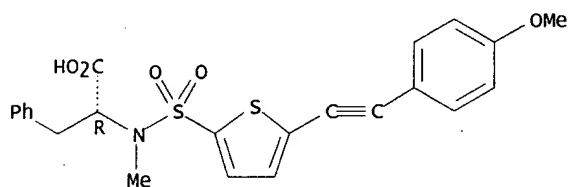
RN 193809-39-1 HCAPLUS  
CN D-Phenylalanine, N-[[5-[(4-fluorophenyl)ethynyl]-2-thienyl]sulfonyl]-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



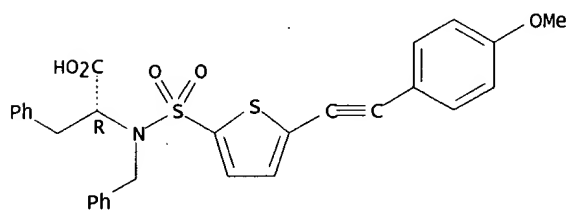
RN 193809-40-4 HCAPLUS  
CN D-Phenylalanine, N-[[5-[(4-methoxyphenyl)ethynyl]-2-thienyl]sulfonyl]-N-  
methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 193809-41-5 HCAPLUS  
CN D-Phenylalanine, N-[[5-[(4-methoxyphenyl)ethynyl]-2-thienyl]sulfonyl]-N-  
(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=&gt; d bib abs hitstr 163 14

L63 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1997:145245 HCAPLUS  
 DN 126:157408  
 TI Preparation of N-(arylcarbonyl or heterocyclylcarbonyl)amino(carboxyalkenyl)bicycloheptane derivatives or analogs thereof and prostaglandin D2 (PGD2) antagonists containing the same  
 IN Ohtani, Mitsuaki; Arimura, Akinori; Tsuru, Tatsuo; Kishino, Junji; Honma, Tsunetoshi  
 PA Shionogi and Co., Ltd., Japan; Ohtani, Mitsuaki; Arimura, Akinori; Tsuru, Tatsuo; Kishino, Junji; Honma, Tsunetoshi  
 SO PCT Int. Appl., 242 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

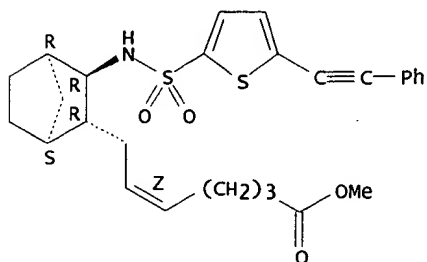
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9700853	A1	19970109	WO 1996-JP1685	19960619
W: AL, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KR, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2225250	AA	19970109	CA 1996-2225250	19960619
AU 9661370	A1	19970122	AU 1996-61370	19960619
AU 714312	B2	19991223		
EP 837052	A1	19980422	EP 1996-918841	19960619
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
CN 1193315	A	19980916	CN 1996-196326	19960619
BR 9608498	A	19990706	BR 1996-8498	19960619
CZ 285870	B6	19991117	CZ 1997-4013	19960619
NO 9705994	A	19980223	NO 1997-5994	19971219
US 6172113	B1	20010109	US 1998-973983	19980422 <--
JP 1995-154575		19950621		
WO 1996-JP1685		19960619		
OS MARPAT 126:157408				
GI For diagram(s), see printed CA Issue.				
AB	Compds. of general formula [I; ring Y = Q - Q3; A = alkylene optionally interrupted with phenylene or hetero atoms and optionally contg. oxo and/or unsatd. bonds; B = H, alkyl, aralkyl, acyl; R = CO2R1, CH2OR2, CONR3R4; R1, R2 = H, alkyl; R3, R4 = H, alkyl, OH, alkylsulfonyl; X1 = single bond, phenylene, naphthylene, thiophenediyl, indolediyl, oxazolediyl; X2 = single bond, N:N, N:CH, CH:N, CH:NN, CH:NO, C:NNHCSNH, C:NNHCONH, CH:CH, CH(OH), CCl:CCl, (CH2)n, C.tplbond.C, NR5, NR5CO, NR5SO2, NR5CONR5, CONR5, SO2NR5, O, S, SO, SO2, CO, oxadiazolediyl, thiadiazolediyl, tetrazolediyl; wherein R5 = H, alkyl; X3 = alkyl, alkenyl, alkynyl, aryl, aralkyl, heterocyclyl, cycloalkyl, cycloalkenyl, thiazolyldene, etc.; Z = SO2, CO; m = 0,1; wherein if the substituents are in the form of rings, they may be optionally substituted] or salts thereof or hydrates thereof are prepd. These compds. are useful as a PGD2 antagonists and thus usable in, for example, a remedy for systemic mastocytosis or systemic mast cell activation disorders, a drug for bronchoconstriction, an antiasthmatic, a drug for allergic rhinitis agent, a drug for allergic conjunctivitis, a drug for urticaria, a remedy for ischemia reperfusion disorders or an antiinflammatory agent. They are particularly useful in the treatment of nasal occlusion. Thus, a bicyclo[2.2.1]heptane deriv. (II; R = Me, R7 = H) was condensed with 2-chlorosulfonyldibenzofuran in the presence of Et3N in CH2Cl2 to give, after sapon., II.Na (R = H, R7 = Q3). I in vitro inhibited the binding of [3H]PGD2 to PGD2 receptor prepn. from human blood platelet fraction with IC50 of 0.003-8.6 .mu.M. A tablet and granule formulation contg. the title compd. (III.1/2Ca) were described.			
IT	186528-86-9P 186528-87-0P RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of amino(carboxyalkenyl)bicycloheptane derivs. as prostaglandin D2 antagonists for disease therapy)			
RN	186528-86-9 HCAPLUS			
CN	5-Heptenoic acid, 7-[3-[[[5-(phenylethynyl)-2-thienyl]sulfonyl]amino]bicyclo[2.2.1]hept-2-yl]-, methyl ester,			

SEARCHED BY SUSAN HANLEY 305-4053

CHOI 09/387,135

[1S-[1.alpha.,2.alpha.(Z),3.beta.,4.alpha.]]- (9CI) (CA INDEX NAME)

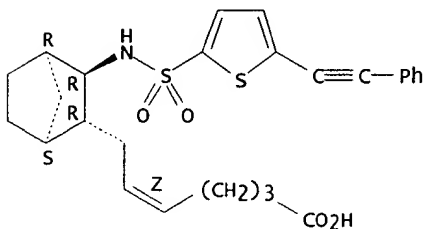
Absolute stereochemistry.  
Double bond geometry as shown.



RN 186528-87-0 HCAPLUS

CN 5-Heptenoic acid, 7-[3-[[[5-(phenylethynyl)-2-thienyl]sulfonyl]amino]bicyclo[2.2.1]hept-2-yl]]-, [1S-[1.alpha.,2.alpha.(Z),3.beta.,4.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

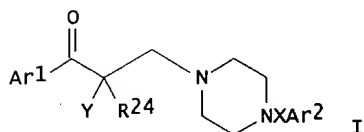




=&gt; d bib abs hitstr 163 15

L63 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1996:467025 HCAPLUS  
 DN 125:114706  
 TI Preparation of substituted (1-aryl-3-piperazin-1'-yl)propanone  
 antibiotics, antimycotics and antineoplastics  
 IN Debernardis, John F.; Kerkman, Daniel J.; Zinkowski, Raymond P.  
 PA Molecular Geriatrics Corporation, USA  
 SO PCT Int. Appl., 115 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9615792	A1	19960530	WO 1995-US15679	19951116
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5658909	A	19970819	US 1994-341481	19941117
CA 2205504	AA	19960530	CA 1995-2205504	19951116
AU 9645954	A1	19960617	AU 1996-45954	19951116
AU 710012	B2	19990909		
JP 10509956	T2	19980929	JP 1995-517112	19951116
US 6075026	A	20000613	US 1997-837598	19970421 <--
PRAI US 1994-341481		19941117		
WO 1995-US15679		19951116		
OS MARPAT 125:114706				
GI				

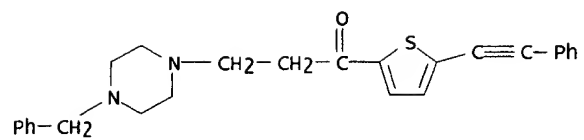


AB The title compds. [I; X = carbonyl, sulfonyl, (un)substituted methylene; Z = N, CH; Ar1, Ar2 = (un)substituted aryl; R24, Y = H; etc.], useful in the treatment of neoplastic diseases and bacterial or fungal infections, and for preventing or decreasing the prodn. of abnormally phosphorylated paired helical filament (PHF) epitopes assocd. with Alzheimer's disease, are prepd. Thus, p-nitroacetophenone was reacted with 1-benzylpiperazine, paraformaldehyde, and concd. HCl, producing 1-(p-nitrophenyl)-3-(4'-benzyl-1'-piperazinyl)-1-propanone dihydrochloride, m.p. 250.degree., which demonstrated a IC50 of 5.0 .mu.M for inhibition of TG3 immunoreactivity in OKA-treated MSN1a cells, vs. approx. 70 .mu.M for chlorpromazine.

IT 179335-34-3P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);  
 PREP (Preparation); USES (Uses)  
 (prepn. of substituted (1-aryl-3-piperazin-1'-yl)propanone antibiotics, antimycotics and antineoplastics)

RN 179335-34-3 HCAPLUS  
 CN 1-Propanone, 1-[5-(phenylethynyl)-2-thienyl]-3-[4-(phenylmethyl)-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)

CHOI 09/387,135



● 2 HCl

=&gt; d bib abs hitstr 163 16

L63 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2001 ACS

AN 1995:995752 HCAPLUS

DN 124:145618

TI Preparation of [3-(1-adamantyl)phenyl]acetylene moiety-containing pharmaceutical and cosmetic compositions

IN Bernardon, Jean-Michel; Charpentier, Bruno

PA Centre International de Recherches Dermatologiques Galderma, (CIRD Galderma), Fr.

SO Eur. Pat. Appl., 26 pp.

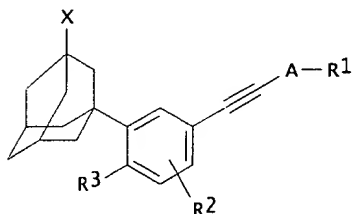
CODEN: EPXXDW

DT Patent

LA French

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 679631	A1	19951102	EP 1995-400737	19950403
	EP 679631	B1	19980506		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	FR 2719044	A1	19951027	FR 1994-5018	19940426
	FR 2719044	B1	19960531		
	AT 165808	E	19980515	AT 1995-400737	19950403
	ES 2120145	T3	19981016	ES 1995-400737	19950403
	ZA 9502975	A	19951221	ZA 1995-2975	19950411
	AU 9516509	A1	19951116	AU 1995-16509	19950418
	AU 674814	B2	19970109		
	NO 9501544	A	19951027	NO 1995-1544	19950424
	CA 2147808	AA	19951027	CA 1995-2147808	19950425
	JP 08092136	A2	19960409	JP 1995-101513	19950425
	JP 2756424	B2	19980525		
	HU 74009	A2	19961028	HU 1995-1166	19950425 <--
	HU 217832	B	20000428		
	BR 9501613	A	19970916	BR 1995-1613	19950425
	RU 2125554	C1	19990127	RU 1995-106684	19950425
	FI 9501983	A	19951027	FI 1995-1983	19950426
	US 5574036	A	19961112	US 1995-429045	19950426
	US 5798354	A	19980825	US 1996-678416	19960702
PRAI	FR 1994-5018		19940426		
	US 1995-429045		19950426		
OS	MARPAT 124:145618				
GI					



AB The title compds. [I; A = (un)substituted 1,4-phenylene, (un)substituted 2,6-naphthalenediyl, pyridinediyl, furandiyl, thiophenediyl, etc.; R1 = H, Me, etc.; R2 = H, halogen, (un)branched alkyl, etc.; R3 = OCH2OCH2CH2OMe, etc.; X = H, halogen] [e.g., 4-[3-(1-adamantyl)-4-methoxyphenylethynyl]benzoic acid, m.p. 307-310.degree.], useful as cardiovascular agents (no data), antirheumatics (no data), skin-care agents (no data), hair preps. (no data), etc. (no data), are prepd. and I-contg. formulations presented.

IT 173191-01-0P 173191-02-1P 173191-03-2P

RL: NUU (Nonbiological use, unclassified); SPN (Synthetic preparation);

THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); USES (Uses)

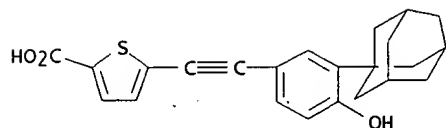
(prepn. of [3-(1-adamantyl)phenyl]acetylene moiety-contg. pharmaceutical and cosmetic compns.)

RN 173191-01-0 HCAPLUS

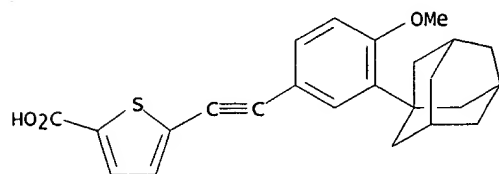
CN 2-Thiophenecarboxylic acid, 5-[(4-hydroxy-3-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-

SEARCHED BY SUSAN HANLEY 305-4053

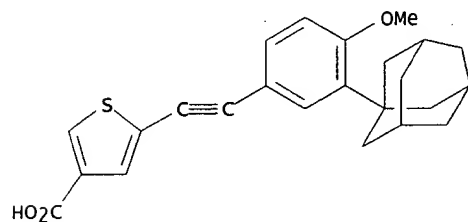
ylphenyl)ethynyl]- (9CI) (CA INDEX NAME)

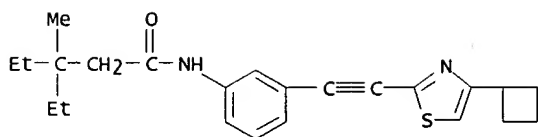


RN 173191-02-1 HCAPLUS  
CN 2-Thiophenecarboxylic acid, 5-[(4-methoxy-3-tricyclo[3.3.1.3.3]dec-1-ylphenyl)ethynyl]- (9CI) (CA INDEX NAME)

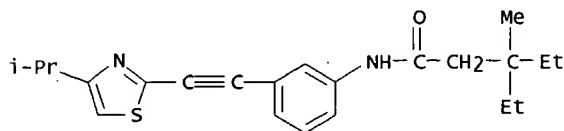


RN 173191-03-2 HCAPLUS  
CN 3-Thiophenecarboxylic acid, 5-[(4-methoxy-3-tricyclo[3.3.1.3.3]dec-1-ylphenyl)ethynyl]- (9CI) (CA INDEX NAME)

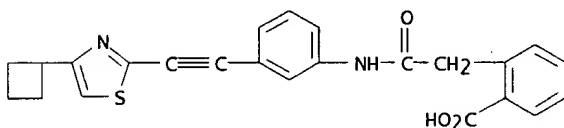




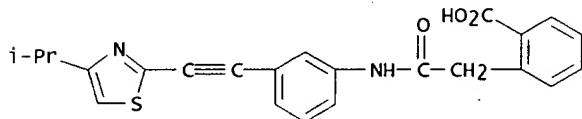
RN 184154-28-7 HCAPLUS  
CN Pentanamide, 3-ethyl-3-methyl-N-[3-[[4-(1-methylethyl)-2-thiazolyl]ethynyl]phenyl]- (9CI) (CA INDEX NAME)



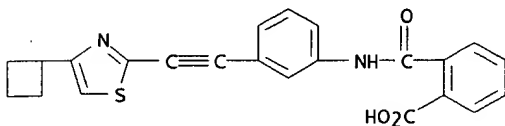
RN 184154-30-1 HCAPLUS  
CN Benzoic acid, 2-[2-[[3-[[4-(1-methylethyl)-2-thiazolyl]ethynyl]phenyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



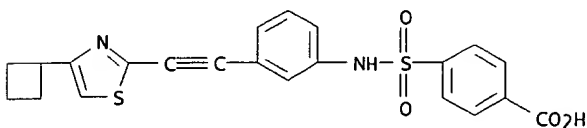
RN 184154-32-3 HCAPLUS  
CN Benzoic acid, 2-[2-[[3-[[4-(1-methylethyl)-2-thiazolyl]ethynyl]phenyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



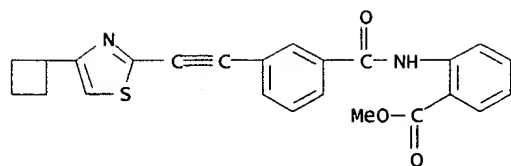
RN 184154-33-4 HCAPLUS  
CN Benzoic acid, 2-[[[3-[[4-(1-methylethyl)-2-thiazolyl]ethynyl]phenyl]amino]carbo-nyl]- (9CI) (CA INDEX NAME)



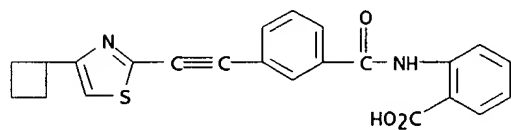
RN 184154-35-6 HCAPLUS  
CN Benzoic acid, 4-[[[3-[[4-(1-methylethyl)-2-thiazolyl]ethynyl]phenyl]amino]sulfo-nyl]- (9CI) (CA INDEX NAME)



RN 184154-52-7 HCAPLUS  
CN Benzoic acid, 2-[3-[[4-(1-methylethyl)-2-thiazolyl]ethynyl]benzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 184154-53-8 HCAPLUS  
 CN Benzoic acid, 2-[[3-[(4-cyclobutyl-2-thiazolyl)ethynyl]benzoyl]amino]-  
 (9CI) (CA INDEX NAME)



=&gt; d bib abs hitstr 154 6

L54 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2001 ACS

AN 1994:701075 HCAPLUS

DN 121:301075

TI Preparation of phosphonic acid derivatives useful for medically treating hyperlipemia

IN Yoshida, Ichirou; Ikuta, Hironori; Fukuda, Yoshio; Eguchi, Yoshihito; Kaino, Makoto; Tagami, Katsuya; Kobayashi, Naoki; Hayashi, Kenji; Hiyoshi, Hironobu; et al.

PA Eisai Co., Ltd., Japan

SO PCT Int. Appl., 363 pp.

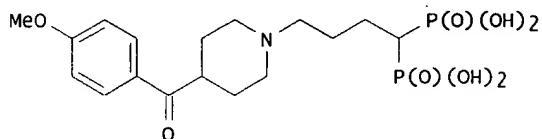
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9420508	A1	19940915	WO 1994-JP354	19940304
	W: AU, CA, CN, FI, HU, JP, KR, NO, NZ, RU, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9461564	A1	19940926	AU 1994-61564	19940304
	EP 688325	A1	19951227	EP 1994-908498	19940304
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	HU 72307	A2	19960429	HU 1995-1944	19940304
	JP 08508245	T2	19960903	JP 1994-519819	19940304
	ZA 9401575	A	19941013	ZA 1994-1575	19940307
	US 5719303	A	19980217	US 1995-530311	19950906
PRAI	JP 1993-46389		19930308		
	WO 1994-JP354		19940304		
OS	MARPAT 121:301075				
GI					



AB 533 Phosphonic acid derivs. RACRBR1P(O)(OR2)(OR3), e.g., I, or their pharmacol. acceptable salts, useful for medically treating hyperlipemia, were prepd. The compds. of the present invention act as effective squalene synthetase inhibitors (test data given).

IT 159270-75-4P

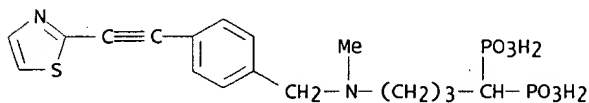
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);

PREP (Preparation); USES (Uses)

(prepn. of phosphonic acid derivs. useful for medically treating hyperlipemia)

RN 159270-75-4 HCAPLUS

CN Phosphonic acid, [4-[methyl[[4-(2-thiazolyethynyl)phenyl]methyl]amino]butylidene]bis-, tetrasodium salt (9CI) (CA INDEX NAME)



● 4 Na